AN INVESTIGATION OF METHODS FOR NEUTRON CROSS SECTION ERROR IDENTIFICATION UTILIZING INTEGRAL DATA

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AN INVESTIGATION OF METHODS FOR NEUTRON CROSS SECTION

ERROR IDENTIFICATION UTILIZING INTEGRAL DATA

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SUMMARY

Uncertainties in nuclear cross section data, in the fast energy range, are a source of appreciable uncertainties in fast reactor design parameters.

Although most investigators realize that crucial information can be obtained from the discrepancies between theoretical and experimental integral data, there exist various fitting procedures, proposed by many international groups, on how to effectively utilize these discrepancies to diagnose the uncertainties in nuclear quantities.

To give a unified treatment of numerous fitting schemes available, a one group study was previously carried out, with the consideration of the k values only. However, other significant questions still need to be investigated, such as how the incorporation of realistic multigroup cross sections, cross section correlation ratios, and the utilization of different types of integral quantities would affect the differential error identification.

This dissertation, in essence a continuation of the previous one group study, considers different fitting schemes, varying the multigroup structure and the choice of integral data, and attempts to determine under what conditions meaningful information on the improvement of cross section data can be obtained.

Basically this study considers four fitting procedures; the first one minimizes an "integral" term, which represents the difference between the experimental and theoretical values of integral parameters. The second

procedure minimizes the integral term subject to a fixed constraint on a "differential" term, which represents the changes in the cross sections used to calculate the integral parameters. The third one minimizes the sum of the integral and the differential term. The fourth procedure minimizes the differential term subject to a constraint on the integral term. By varying the constraint size of the differential term in the second procedure, this work offers a rigorous treatment of all fitting procedures on a common basis.

This study, which involves investigation of up to four energy groups, not only considers the influence of various errors, both statistical and systematic, on the error identification, but also tries to give answers to many unsettled queries such as the optimal choice of the weighting factor between the integral and the differential term in the third procedure, the optimal choice of the constraint size on the cross section term, the relationship between the degree of error identification and the ratio of integral to differential data, and the effects of considering and ignoring cross section correlation ratios in a fitting.

As an improvement of the previous one group study, this study first uses a more systematic method of introducing cross section errors, and then employs a new figure of merit for a better interpretation of the results from error identification.

The results obtained from the first fitting procedure which only minimizes the integral term are not very satisfactory. If a highly overdetermined system (that is, the number of integral data is much larger than that of differential data) is used, satisfactory results can be obtained with this fit.

For the second fitting procedure, which has a constraint on the variation of the differential data, there exists an optimal constraint size which will give the best results when compared with the other fitting procedures. An empirical choice, which often lies in the vicinity of the optimal constraint size and gives the best results for error identification, is determined from the results in this study.

For the third fitting procedure, which minimizes the sum of the integral and the differential terms, there is an optimal weighting factor between these two terms for the best results in the error identification. For the 2, 3, and 4 group cases studied, the weighting factor of 1/G, where G is the number of energy groups, yields better results than the choice of 1.0. In a realistic situation, one has no prior knowledge of the optimal weighting factor; but based on the previous statement and the fact that such a factor will tend to prevent the relative overall weight of the differential data from becoming increasingly large as the number of energy groups is increased, the 1/G factor appears to be a better choice.

For the fitting procedure with a constraint on the integral data, significant error identification is possible if the statistical errors of the experimental integral data are not underestimated. However, this procedure usually gives results which are inferior to those of either the second procedure with the empirical choice of the constraint, or the third procedure with a 1/G weighting factor.

For the cases considered, it appears that good error identification is possible if the systematic errors are moderate in size.

Based on the results in this study, one generally obtains better

overall error identification if one uses both the k values and reaction rate ratios instead of just one type of integral data.

In general the error identification by any fitting procedure improves if the statistical errors of the experimental integral data decrease or if the number of integral data increases, as one would expect.

Finally one finds that when using relatively accurate k values and reaction rate ratios, one can obtain significant error identification for the cases considered (e.g. many 4 group cases) whether cross section correlation ratios are included in the fit or not; the inclusion of such correlation does not significantly improve the error identification. However, as the accuracy of the experimental integral data decreases, the inclusion of correlation tends to improve the error identification.

CHAPTER I

NATURE OF THE PROBLEM

The energy crisis is one of the most discussed subjects in this era of vast technological advancement. While the power demand at least doubles every ten years in this country, it is an inevitable truth that the reserves of economically and practically available fossil fuel are not sufficient to satisfy this rapidly increasing need. Considering the fact that the economic utilization of both fusion and solar energy is still uncertain, it appears that the only imminent alternative available to mankind is to utilize nuclear energy in the most sensible manner.

With the successful realization of converting fertile material into fissile fuel, there is considerable interest in obtaining more accurate design parameters for more effective operation of fast breeder reactors. However, in many cases, the nuclear cross section data evaluated from the microscopic measurements are presently unknown to the desired accuracy which is necessary for the calculation of fast reactor parameters.

A survey on the measured cross section data available at present indicates that above a few hundred eV, which is the energy range of most interest to the fast systems, the uncertainties on these values for the important isotopes such as Pu-239 and U-238 are of the order of ten percent.[1]

These large uncertainties would definitely affect the accuracy of the design parameters. One of the conspicuous examples is the uncertainty

of the measured σ_c of U-238,[2] which might contribute in the range from 1 to 100 keV an uncertainty of 0.06 in the calculated breeding ratio and 0.015 for any higher energy. The measurements of α, the capture to fission ratio, are sometimes in large disagreement. For instance, α of Pu-239 below 15 keV used to yield considerable disagreement between various measurements; though it has been experimentally resolved during recent years, its 20% uncertainty is still too high for reducing the uncertainty of the fuel cost to an acceptable value. Even in the case of the most popular standard cross section, σ_f of U-235, the discrepancy between various experimental results of White and that of Poenitz, which is much lower, is still unsettled.[1]

The goal for 1975 demands the fuel cost for a 1000 MW(e) reactor be reduced from the present uncertainty of 0.13 mill/KW(e)h to 0.03 mill/KW(e)h.[3] This unquestionably implies more accurate information on cross sections, which might possibly require the reduction of the error in σ_c and σ_f of U-238 and Pu-239 to 2% in the energy range of interest.

In this country and many countries abroad, most work associated with breeder development utilizes Brookhaven National Laboratory's ENDF/B cross section library as their tool. However, many studies have shown that this set contains significant errors. For example, one experimental study[4] shows ENDF/B version I underpredicts the neutron spectrum below 2 keV and above 2 MeV, and another study[5] shows ENDF/B version I underestimates k in many assemblies by 2% whereas the version II, despite the effort to update the first version, is made worse and underestimates k by 3 to 5%. The quandary is a clear indication that the problem of adjusting cross sections is by no means trivial. Due to some data adjustment utiliz-

ing k values, the accuracy of ENDF/B version III is good for criticality calculations; nevertheless, the cross section adjustments to make k values calculated better were not made in a particularly systematic manner; there may still exist compensating errors in the cross sections important for k values. Furthermore, the application of ENDF/B version III in calculations related to reactor economy and reliability is stil nebulous[6]; for instance, one study[7] shows it over-predicts the $\sigma_c^{U\text{-}238}/\sigma_f^{U\text{-}235}$ reaction rate ratio by 10 to 15%. Thus many designers feel there indeed exists a need for more sophisticated studies which consider data fitting of reaction rate ratios and other integral data in addition to k values to improve cross sections.

In recent years the number of fast critical assemblies around the world has multiplied significantly. With the increasing amount of accurate integral data available from the fast criticals, the notion of utilizing these data with modern high-speed computers in a constructive manner to predict and improve the differential nuclear cross sections is more justified.

Previous Investigation and Present Status

Fitting Procedures

At the 1966 Argonne Conference on fast critical assemblies, four papers by Pendlebury,[8] Cecchini,[9] Baker,[10] and Pazy[11] were discussed. Later at the 1969 London Conference on fast reactor design, further developments of fitting schemes were reported in papers by Ballance and Pendlebury,[12] Rowlands and Macdougall,[13] Barré,[14] and Bitelli et al.[15] The underlying theme of all these works is that the deviation between the

experimental and the theoretical integral data should be utilized to adjust cross sections properly. The theory of these data fittings is based on the principle of least squares; the fundamental difference between fitting schemes lies in the emphasis on the integral or the differential data as determined by the choice of the weighting factor between these quantities, or the appropriate constraint on the integral or the differential data.

Perturbation Theory

Weinberg[16] first exploited perturbation theory to investigate the change in k_{eff} for some reactor system for some cross section change. There exists considerable interest in finding the variation of other crucial parameters of design, such as the breeding ratio, reactivity worths, and others, since the "normal" perturbation theory could not calculate changes in such parameters. Finally Usachev published a paper[17] in which the method of successive approximation was used to deal with the variation of the breeding ratio and other ratios of linear functionals of the real flux. Since then great progress in this field has been made by a group of Italian scientists headed by Gandini.[18]

Gandini first modified Usachev's approach to include the ratio of linear functionals of the adjoint flux.[18] The formula he established for the ratio of this nature was applicable to the evaluation of the change of neutron source worth due to changes introduced to a fast reactor with neutron sources. Then in a later paper[19] he extended this method and presented a generalized perturbation theory for evaluating the ratio of two bilinear functionals of both real and adjoint flux. The perturbation expressions he derived may be used to calculate the sensitivity coefficients for reactivity worths, reactivity ratios, and prompt neutron lifetimes.

Zero Dimension One Group Model

A zero dimension one group model has been developed by Ott, Pond, and Kallfelz[20,22] for comparison of various fitting schemes which attempt to identify errors in the microscopic data employing the integral discrepancies.

The model is based upon diffusion theory and uses a buckling term to replace the dimensional leakage of neutrons. When considering fairly large fast systems such as the Demonstration Plant Benchmark Critical Assemblies,[21] the zero dimension model is sufficient and the diffusion theory is a good approximation to the exact transport theory as long as one is studying the reactor processes such as central worths which occur in the core center; also, k sensitivity calculations with this model are good for a single core region. Furthermore, for the gedanken experiments, which are used in this study to investigate the fitting procedures themselves rather than the reactor parameters, the result from the simple model used in this study can be considered exact. (A gedanken experiment is a theoretical experiment in which one assumes one already knows the answers, namely, the errors in the differential data, so that one can use the known answers to study various fitting procedures.) One energy group of neutrons was adopted for the study in reference 20. Since the introduction of the energy or the space dependence complicates the issue, any method which does not yield meaningful results for the simple model will surely not give better results for the more complex case. To obtain more insight into the problem, the initial studies thus used the least complex model.

Four Basic Fitting Procedures

The four fitting procedures investigated in the previous one group study[20,22] can be expressed in the following algebraic forms.

(1) Procedure No. 1, the standard least square, no constraint fit, finds u_k which minimizes

$$\sum_n \left[\left(\frac{1}{S_n^I} \right)^2 \left(\sum_k H_{kn} u_k + \Delta I_n \right)^2 \right]$$

where u_k is the unknown, the identified change, in the group cross section k

ΔI_n is the difference between the theoretical and the experimental results for the n^{th} integral value

H_{kn} is the change of the n^{th} theoretical value due to a unit change in the cross section error u_k; H_{kn} is called the sensitivity coefficient

S_n^I is the standard deviation of the experimental integral data I_n.

(2) Procedure No. 2, the ellipsoidal fit, finds u_k which minimizes

$$\sum_n \left[\left(\frac{1}{S_n^I} \right)^2 \left(\sum_k H_{kn} u_k + \Delta I_n \right)^2 \right]$$

subject to the constraint $$\sum_k \frac{u_k^2}{\omega_k^2} \leq 1$$

where $\omega_k = \beta S_k^\sigma$

β is some scale factor, and

S_k^σ is the standard deviation of cross section k.

(3) Procedure No. 3, the combined fit, finds u_k which minimizes

$$\sum_n \left[\left(\frac{1}{S_n^I}\right)^2 \left(\sum_k H_{kn} u_k + \Delta I_n \right)^2 \right] + \gamma \left[\sum_k \frac{u_k^2}{(S_k^\sigma)^2} \right]$$

where γ is a weighting factor.

(4) Procedure No. 4, the fixed square fit, finds u_k which minimizes $\sum_k \frac{u_k^2}{(S_k^\sigma)^2}$ subject to constraint

$$\left| \sum_n \left[\left(\frac{1}{S_n^I}\right)^2 \left(\sum_k H_{kn} u_k + \Delta I_n \right)^2 \right] \right| = N$$

where N is the total number of integral data used in the fit.

To facilitate the future discussion on the theories behind the data fitting, the four fitting procedures are reproduced here in matrix formalism, using the following definitions:

u is a k x 1 vector with its element u_k.

y is an n x 1 vector with its element ΔI_n.

H is an n x k matrix with its element H_{kn}.

P is a k x k diagonal matrix with its element $p_{ii} = (S_i^\sigma)^2$.

Q is an n x n diagonal matrix with its element $q_{ii} = (S_i^I)^2$.

W is a k x k diagonal matrix with its element $w_{ii} = \omega_i^2$.

u_k, ΔI_n, H_{kn}, S_i^σ, S_i^I, and ω_i are defined on the preceding page.

Then procedure No. 1, the standard least square, no constraint fit, is to find u which minimizes $(y-Hu)^T Q^{-1} (y-Hu)$, where T stands for the transpose operation. (1)

Procedure No. 2, the ellipsoidal fit, is to find u which minimizes $(y-Hu)^T Q^{-1} (y-Hu)$ subject to $u^T w^{-1} u \leq 1$. (2)

Procedure No. 3, the combined fit, is to find u which minimizes

$$(y-Hu)^T Q^{-1}(y-Hu) + \gamma\, u^T P^{-1} u \qquad \text{where } \gamma \text{ is a weighting factor.} \tag{3}$$

Procedure No. 4, the fixed square fit, is to find u which minimizes $u^T P^{-1} u$ subject to $\left|(y-Hu)^T Q^{-1}(y-Hu)\right| = N$ where N is the total number of integral data. (4)

The Zero Dimension One Group Model

The fitting formula of the nuclear cross section errors for the one group, space independent case was derived in detail in the previous one group study.[22] The set of the linear equations obtained satisfies the formalism in procedure no. 1, which is the standard least square, no constraint fit.

The Proposed Work and Its Objective

A general mathematical study has been made of various fitting procedures. The fitting procedures may or may not include certain constraints; for those which involve constraints, the method of La Grange multipliers on both the differential and the integral values was used to apply these constraints.

The investigation involved numerical studies in which assumed errors were introduced into the cross sections, and error identification was attempted with various fitting procedures, using gedanken integral experiments.

The objective of this work is to evaluate the situations under which the data of integral experiments in fast critical assemblies might be utilized to give meaningful identification of errors in differential neutron

cross section value. The relevant conditions which were not considered in the previous one group study[22] and have been considered in this study are listed as follows.

1. The energy dependence up to 4 groups has been incorporated in the cross section data.

2. Both k values and other integral parameters, namely, the reaction rate ratios, have been used in data fitting.

3. The sensitivity coefficients of both the k and the reaction rate ratios have been calculated utilizing the normal and the generalized perturbation theories.

4. A more systematic method of introducing cross section errors has been employed than that used in the previous study[22] to insure that these errors are statistical in nature.

5. A new figure of merit has been developed for a better interpretation of the performance of a fitting procedure in error identification.

6. A thorough theoretical analysis of the solutions of the fitting schemes has been performed.

7. The estimators for the standard deviations of the cross section errors have been derived vigorously.

8. The pseudoinverse has been used in solving the underdetermined case of the standard least square fit.

9. The effects of considering and ignoring cross section correlation ratios have been investigated in data fitting.

10. The empirical constraint size for the cross section data has been determined to yield the best results in error identification.

11. Two possible choices of the weighting factor between the integral and the differential data have been investigated, and the choice which gives the most meaningful results from data fitting has been determined.

CHAPTER II

THEORIES OF DATA FITTING

Linear Model of Data Fitting

In many fields of science and engineering, one often has to use data fitting to deal with various estimation problems.

In the field of reactor physics, one is confronted with the following estimation problem:

Given a linear model[23]

$$y = Hu + \epsilon \tag{5}$$

where

y, u, and H are defined in the preceding section and

ϵ is an n x 1 random vector of discrepancies due to the error in experimental integral data,

one wishes to estimate the unknown u.

To attack this interesting problem, one often makes some reasonable assumptions[23] about u and ϵ.

The first assumption is

$$Eu = 0$$

where E denotes taking the expected value.

The second is

$$E(\epsilon\epsilon^T) = Q$$

where Q is defined in the preceding section.

Since there exist many criteria of selecting an estimator of u, the most logical choice is to select the estimator with both the property of unbiasedness and minimum variance. The general solution of such an estimator is based on the theory of least squares.

The Theory of Least Squares

The concept of least squares is based on finding the estimator $\hat{u}$ which minimizes the expression

$$||y - Hu||^2$$

where $||\ ||$ is the Euclidean norm,

y is a known vector,

H is a known matrix,

and $\hat{u}$ is the estimator for the unknown vector u.

In the field of statistics, the estimator u thus derived is called the least squares estimator.[24]

From the geometric consideration, the solution of the least squares estimator generally involves the idea of a projection.[24] The definition of a projection is as follows:

> A linear operator P on a finite dimensional vector space is called a projection if P is idempotent; that is $P^2 = P$.

There are various types of projection. The particular type related to the solution of the least squares estimator is the orthogonal projection[24] which has the additional property of symmetry. That is, a projection P is orthogonal if $P = P^T$.

It can be shown that the least squares estimator $\hat{u}$ can be obtained by projecting y orthogonally into the column space of H. That is,

$$H\hat{u} = P_H y,$$

where P_H is the projection matrix into the column space of H.

The advantage of the least squares solution was shown by Gauss-Markov theorem[23] which claimed that under the condition of the linear model specified in (5) if $\hat{u}$ is the least squares estimator of u, then $\hat{u}$ is also the unique minimum variance, unbiased linear estimator of u.

Since the objective of the data fitting is to find the unbiased minimum variance linear estimator, one should use the least squares fitting to find such an estimator simply because the least squares fitting is the easiest and thus the most effective method.

Four Fitting Procedures

From the formalism of the four fitting procedures, one can readily perceive that the standard least square, no constraint fit and the combined fit, each of which has no constraint, are easier to tackle than the other fitting schemes.

Since the ellipsoidal fit and the fixed square fit have a similar form, it is instructive to study the solution of the ellipsoidal fit so that the solution of the fixed square fit can be derived from the same line of reasoning. Consequently, the problem one confronts is that of the typical nonlinear program; that is, finding u which minimizes f(u) subject to $g(u) - 1 = 0$.

Generally one can transform it into an equivalent problem of finding the critical points of F, which is given by

$$F(u,\lambda) = f(u) + \lambda[g(u) - 1]$$

where λ is some unknown La Grange multiplier.

The definition of a critical point and the validity of the transformation are discussed in Appendix A.

The next logical approach is to take the partial derivative of F with respect to u first, and then λ, and finally set both expressions to zero to solve for u and λ.

Before one proceeds on this course, one should obtain a few useful working formulas associated with partial derivatives of matrices[25]:

$$\nabla_u(B^T u) = B$$

$$\nabla_u(u^T c) = c$$

$$\nabla_u(A^T S A) = 2(\nabla_u A^T)\, SA$$

where

A is an n x 1 vector whose elements are functions of u,

B is an n x 1 vector whose elements are not functions of u,

S is an n x n symmetric positive definite matrix whose elements are not functions of u,

c is an n x m matrix whose elements are not functions of u,

and ∇_u is an n x 1 operator vector which denotes taking partial derivatives with respect to u.

As was discussed in the previous section, the ellipsoidal fit is to find u which minimizes $(y-Hu)^T Q^{-1}(y-Hu)$ subject to $u^T W^{-1} u \leq 1$.

To transform it into an equivalent problem, one creates a function F such that

$$F = (y-Hu)^T Q^{-1}(y-Hu) + \lambda(u^T W^{-1} u - 1) \qquad (6)$$

where λ is some unknown La Grange multiplier.

Taking the partial derivative of F with respect to u, setting it to zero, and utilizing the set of the working formulas, one obtains

$$H^T Q^{-1} y = (H^T Q^{-1} H + \lambda W^{-1}) u$$

Taking the partial derivative of F with respect to λ, one obtains the original constraint condition

$$u^T W^{-1} u = 1$$

Thus $\hat{u}$ which solves (6) is

$$\hat{u} = (H^T Q^{-1} H + \lambda W^{-1})^{-1} H^T Q^{-1} y$$

which satisfies

$$\hat{u}^T W^{-1} \hat{u} = 1$$

The problem of solving these two sets of equations simultaneously is apparently iterative. Due to the nonnegative definite quadratic form of the function to be minimized and its constraint (6), the La Grange multiplier for the solution will always be positive (see Appendix A), so the actual mechanics of the first few iterations on u and λ by computer programming is on a trial and error basis. However, one observes that as λ increases, the corresponding diagonal elements of the inverse of the matrix $(H^T Q^{-1} H + \lambda W^{-1})$ would tend to decrease; this results in a decrease

in u which would reduce the constraint value accordingly.

What has been discussed is the solution of the ellipsoidal fit which has the similar form as that of the fixed square fit; furthermore, the solution of the standard least square, no constraint fit, and the combined fit can be derived from that of the ellipsoidal fit with a slight modification.

Variance Covariance of the Estimator

The variance of a random variable can be regarded as some measure of the uncertainty of that variable; thus often in the statistical analysis one seeks the variance of the estimator to shed some light on the accuracy of the outcome from the data fitting.

In the case of a random vector u, the definition of the related variance covariance matrix ψ is given by[23]

$$\psi = E[(u - Eu)(u - Eu)^T] \tag{7}$$

which can be simplified into[23]

$$\psi = E(uu^T) - (Eu)(Eu)^T$$

The derivation of ψ for the ellipsoidal fit will be shown below, and the expressions for the other three procedures adhere to the same approach. However, one should first state a working formula for ψ to facilitate further discussion.

Under the conditions specified in the linear model of (5) and if

the estimator $\hat{u}$ is of the form $\hat{u} = VQ^{-1}y$, then the variance covariance ψ is

$$\psi = VQ^{-1}V^T \tag{9}$$

where $V = (H^TQ^{-1}H + \lambda W^{-1})^{-1}$.

Substituting (9) into (8), one establishes

$$\psi = VH^TQ^{-1}HV^T$$

Since V which is the inverse of the sum of two symmetric matrices is also symmetric, then ψ can be rewritten into a neater form

$$\psi = (HV)^TQ^{-1}(HV)$$

Furthermore, note that Q^{-1} is a positive diagonal matrix and thus can be expressed by

$$Q^{-1} = (Q^{-1/2})^T(Q^{-1/2})$$

where $Q^{-1/2}$ is also a diagonal matrix with each element equal to the square root of the associated element in Q^{-1}.

Finally one concludes that

$$\psi = (Q^{-1/2}HV)^T(Q^{-1/2}HV)$$

Overdetermined and Underdetermined Systems

The previous discussion is based on the tacit assumption that there exists more integral data than the unknown cross section errors; that is, $K < N$ for the overdetermined case. However, in realistic situations due to the difficulty in generating a lot of integral data in a limited number of physical assemblies, the number of unknown nuclear errors is often larger than that of integral quantities involved, if more than several energy groups are considered. Thus one needs to examine the linear model and the solution of each fitting scheme in a more discrete manner.

Since $K > N$ for the underdetermined case, the rank of H, the coefficient matrix, is always less than k. Using this condition, the rank of $H^T Q^{-1} H$, which appears in the solution of each fitting scheme, is also less than k.

This leads to the unfortunate fact that the solution of the standard least square, no constraint fit for the overdetermined case does not apply to the underdetermined case. However, for the other three procedures, the addition of another term (caused by inclusion of the present cross section values in the fit), which is always a positive diagonal matrix, to $H^T Q^{-1} H$ in the solutions will definitely remove the linear dependence of the column vectors of $H^T Q^{-1} H$; therefore, the matrix inversion is possible. The inclusion can be interpreted as the inclusion of more experimental data (cross sections) in the fit.[8]

As for the standard least square, no constraint fit, the meaning of obtaining the optimal solution can be redefined as follows:

Find, among all the solutions u which minimize $(Hu-y)^T Q^{-1} (Hu-y)$, the particular u which also minimizes $u^T P^{-1} u$.

As a word of caution, one should realize that the solution u which first minimizes $(Hu-y)^T Q^{-1}(Hu-y)$ and then minimizes $u^T P^{-1} u$ is not the same as the u which minimizes $(Hu-y)^T Q^{-1}(Hu-y) + u^T P^{-1} u$ in the combined fit.

To attack the underdetermined case of the standard least square, no constraint fit, one has to use the pseudoinverse of a matrix.

H^+ is defined to be the pseudoinverse of a matrix H if H^+ satisfies the following relations:

$$HH^+H = H$$
$$H^+HH^+ = H^+$$
$$(H^+H)^* = (H^+H)$$
$$(HH^+)^* = (HH^+)$$

where * denotes the operation of conjugate transpose.

From the above definition of the pseudoinverse, the following two results can be derived[27]:

1. $(H^+)^+ = H$
2. $(H^+)^T = (H^T)^+$

Two of the important theorems associated with the pseudoinverse are listed here without proof.

Theorem 1[28]: For any matrix H,

$$H^+ = \lim_{\delta \to 0} (H^T H + \delta^2 I)^{-1} H^T$$

The application of the pseudoinverse to the solution of the linear system of equations is stated in the next theorem.

Theorem 2[27]: Given a system of linear equations

$$Hu = y$$

where H, y are known matrices, and

u is an unknown vector,

the solution of $\hat{u}$ given by

$$\hat{u} = H^{+}y,$$

where $\hat{u}$ always satisfies the following two criteria:

1. $||H\hat{u} - y|| \leq ||Hu-y||$ for any u

2. If $||H\hat{u} - y|| = ||Hu - y||$

   then $||\hat{u}|| \leq ||u||$

   where $||\ ||$ refers to the norm in the Euclidean space.

The property of the minimum norm of u is often referred to as the minimum biasedness.[24]

To apply Theorem 2 to the underdetermined case of the standard least square, no constraint fit, one first defines a new vector L[24] such that

$$L = P^{-1/2}\hat{u}$$

The function to be minimized in the standard least square, no constraint fit can be transformed into

$$(Hu-y)^{T}Q^{-1}(Hu-y) = (HP^{1/2}L-y)^{T}Q^{-1}(HP^{1/2}L-y)$$

Thus the solution for L is

$$L = (Q^{-1/2}HP^{1/2})^{+}Q^{-1/2}y$$

Using the definition of L, the solution of $\hat{u}$ is

$$\hat{u} = P^{1/2}(Q^{-1/2}HP^{1/2})^{+}Q^{-1/2}y \tag{10}$$

Furthermore, utilizing the identity that for any matrix A,

$$A^{+} = (A^{T}A)^{+}A^{T} \tag{11}$$

the alternate expression for $\hat{u}$ is

$$\hat{u} = P^{1/2}[(HP^{1/2})^{T}Q^{-1}(HP^{1/2})]^{+}(HP^{1/2})^{T}Q^{-1}y \tag{12}$$

The proof of the identity (11) is shown in Appendix E.

In the actual process of computer programming, (12) is more advantageous than (10) in that the pseudoinverse of the symmetric matrix $(HP^{1/2})^{T}Q^{-1}(HP^{1/2})$ will also be symmetric, one of the quick checks on the accuracy of the pseudoinverse operation; moreover, this symmetric matrix is k by k which will occupy less memory storage than the n by k matrix $Q^{-1/2}HP^{1/2}$.

The solutions for the least square estimators and their variance covariance matrices for all four fitting procedures with overdetermined or underdetermined cases are listed in Appendix D.

As a final note, the idea of projection can be extended to the underdetermined case of the standard least square, no constraint fit. The projection matrix[27] in such case is

$$P = HH^{+}$$

which can also incorporate the expression for the overdetermined case.

Classical Perturbation Theory[29]

Time independent neutron diffusion can be described by[29]

$$M\varphi = 0 \tag{13}$$

where $M = F/k - L$,

F is the production term,

L is the loss term,

k is the multiplication constant, and

φ is the flux.

The corresponding adjoint equation is

$$M^{*}\varphi^{*} = 0$$

where $M^{*} = F^{*}/k - L^{*}$,

F^{*} is the transpose of F,

L^{*} is the transpose of L, and

φ^{*} is the adjoint flux.

If one introduces a perturbation to the system, the perturbed diffusion equation is

$$M'\varphi' = 0 \tag{14}$$

where $M' = F'/k' - L'$, and

$'$ denotes the perturbed condition.

Multiplying (13) by φ^*, one can obtain an expression for k which can be shown to be stationary to first order terms in φ and φ^*,

$$k = \frac{<\varphi^*, F\varphi>}{<\varphi^*, L\varphi>} \tag{15}$$

where $<,>$ is the inner product.

Multiplying (14) by φ^* and integrating over all variables, one can also obtain the expression for k'

$$k' = \frac{<\varphi^*, F'\varphi'>}{<\varphi^*, L'\varphi'>} \tag{16}$$

Since the definition of $\frac{\delta k}{k}$ is

$$\frac{\delta k}{k} = \frac{k'-k}{k} \tag{17}$$

one can substitute (15) and (16) into (17). Because of the stationary property of (15), one can replace φ' by φ and obtain an expression which is accurate to first order, i.e., "first order perturbation theory":

$$\frac{\delta k}{k} = \frac{<\varphi^*, (\delta F)\varphi> - k<\varphi^*, (\delta L)\varphi>}{<F\varphi, \varphi^*>}$$

where $\delta F = F' - F$, and

$\delta L = L' - L$.

Generalized Perturbation Theory[17,19]

The reaction rate ratios of interest to the reactor physicist can be expressed by

$$R = \frac{I_1}{I_2} = \frac{< \varphi, f_1 >}{< \varphi, f_2 >} \tag{18}$$

where f_1 and f_2 are some cross sections as functions of space and energy.

One observes that a perturbation of nuclear parameters introduced into the steady state system will not only produce a perturbation δM in the diffusion operator M, but also a perturbation $\frac{\delta R}{R}$, due to changes in φ, and possible changes in f_1, and f_2.

The appropriate perturbation equation Usachev[17] derived is

$$\frac{\delta R}{R} = < \varphi', \delta g > + < \psi^*, (\delta M)\varphi' > \tag{19}$$

where φ' is the perturbed flux

$$\delta g = \frac{\delta f_1}{I_1} - \frac{\delta f_2}{I_2}$$

$$\psi^* = \sum_{i=1}^{\infty} \psi_i^*$$

ψ_i can be solved by the recurrence equations

$$L^*\psi_1^* = g = \frac{f_1}{I_1} - \frac{f_2}{I_2}$$

$$L^*\psi_i^* = \frac{F^*}{k}\psi_{i-1}^* \qquad \text{for the iteration index } i = 2, 3, \ldots$$

The first term in (19) is the "direct effect," while the second term is the "indirect effect" which gives the influence of changes in φ. This second term is still accurate to first order terms if φ' is replaced by φ. This expression will be discussed on page 39.

CHAPTER III

METHOD OF ATTACK

Description of Assemblies

The basic fifty assemblies employed in this study are shown in Table 1 and were derived from the previous one group study.[20] Assemblies 1 to 10 were originally used in similar data fitting schemes by Küchle, Ott, and Schroeter.[30]

The fifty assemblies[22] contain U-238 or Pu-240, the fissile isotopes Pu-239 or U-235, the isotopes Fe, Cr, and Ni, and deuterated polyethylene, D_2C, for spectral shaping. The ratio of the leakage to the absorption was found to be approximately the same for the first ten assemblies. The other forty assemblies, which essentially contain different number densities of various isotopes similar to those present in the first ten assemblies, are designed to have similar spectra to those of the first ten assemblies.

Table 1. Assembly Descriptions in Percents of Volume[20]

Assembly	Pu-239	Pu-240	U-235	U-238	Fe	Ni	Cr	D_2C
1	8			60	20			12
2	6			54	30			10
3	6			36	48			10
4	6			36	30			28
5	4			12	64			20
6	3			5	72			20

Table 1. Continued

Assembly	Pu-239	Pu-240	U-235	U-238	Fe	Ni	Cr	D_2C
7	5			25	50			20
8	9			72				19
9	6			66	10			18
10	6			20	54			20
11	8			60	8	7	5	12
12	6			54	12	10.5	7.5	10
13	6			36	9.6	19.2	19.2	10
14	6			36	22.5	1.5	6	28
15	4			12	48	3.2	12.8	20
16	3			5	39.6	14.4	18	20
17	5			25	27.5	10	12.5	20
18	9			72				19
19	6			66	2	4	4	18
20	6			20	32.4	16.2	5.4	20
21			8	60	20			12
22			6	54	30			10
23			6	36	48			10
24			6	36	30			28
25			4	12	64			20
26			3	5	72			20
27			5	25	50			20
28			9	72				19
29			6	66	10			18
30			6	20	54			20
31	8	2		58	20			12
32	6	3		51	30			10
33	6	2		34	48			10
34	6	3		33	30			28
35	4	1		11	64			20
36	3	1		4	72			20
37	5	3		22	50			20

Table 1. Concluded

Assembly	Pu-239	Pu-240	U-235	U-238	Fe	Ni	Cr	D_2C
38	9	2		70				19
39	6	3		63	10			18
40	6	2		18	54			20
41	8			60		20		12
42	6			54		30		10
43	6			36		48		10
44	6			36		30		28
45	4			12		64		20
46	3			5		72		20
47	5			25		50		20
48	9			72				19
49	6			66		10		18
50	6			20		54		20

Outline for Data Fitting

The underlying theme of data fitting is to study conditions under which errors in the microscopic cross sections can be best identified by fitting the theoretical integral data to their experimental values. This study, which considers both errors in microscopic data and those in integral data, with energy dependence, is essentially a theoretical simulation of data fitting schemes.

In the simulated experiments both the errors in the cross sections and the errors of the experimental integral data are introduced in a random manner. Thus, the outcome of the simulated fitting is to identify the known introduced cross section errors by means of various fitting schemes. The following outline of consecutive steps in executing data fitting is

similar to that in the previous one group study.[22]

1. Perform a spectrum calculation and evaluate the critical buckling for every assembly.

2. Use each spectrum and collapse the 26 ABBN[31] cross sections into a few preassigned broad groups. Thus, for each assembly there is a set of spectrum averaged cross sections which can be considered the known "true" values.

3. Evaluate the typical errors or the standard deviations of the broad group constants.

4. Evaluate the typical errors or the standard deviations of the experimental integral data.

5. Perform random sampling to obtain f_σ, the fractional value of cross section error. The product of the fractional value, f_σ, and its related standard deviation, S^σ, are introduced as the error in the true cross section. This error, which is the difference between the "theoretical" and the true cross section, will be employed as the unknown for the fitting scheme. That is,

$$u_{intro} = S^\sigma * f_\sigma = \sigma_{th} - \sigma_{true}$$

where f_σ is the randomly sampled fractional value,

u_{intro} is the introduced unknown error,

S^σ is the standard deviation of cross section,

σ_{th} is the theoretical cross section, and

σ_{true} is the true cross section.

6. Use the true cross section set to perform the calculation of the true integral data in every assembly and at the same time evaluate the sensitivity coefficients for different cross sections.

Note that in an actual case, the sensitivity coefficients will be calculated using the theoretical cross sections, not the true values. For this gedanken study, as long as the same sensitivity coefficients are used to solve for the errors in a fitting as are used for calculating the introduced errors, the study of various fitting procedures is consistent.

7. Perform a random sampling to obtain f_I, the fractional value of the error in the experimental integral data. The product of f_I, the fractional value, and the associated assumed statistical error in the experimental integral data, S^I, is introduced as the statistical variation of the experimental error in measuring the integral data. This statistical variation of the experimental error gives the difference between the true integral data and the experimental integral data. That is,

$$f_I S^I = I_{true} - I_{ex}$$

where I_{ex} are the experimental integral data,

I_{true} are the true integral data,

f_I is the randomly sampled value (f_I can be positive or negative),

and S^I is the statistical error in the I_{ex}.

Thus the "experimental" integral data are obtained from the difference between the true integral data and the statistical variation of the experimental error. That is,

$$I_{ex} = I_{true} - f_I S^I$$

8. Evaluate the difference between the theoretical and the experimental integral data. This difference can be expressed by the sum of the influence of the cross section errors and some statistical variation of the experimental error in measuring the integral data. That is,

$$I_{th} - I_{true} = \Sigma Hu_{intro}$$

and

$$I_{th} - I_{ex} = \Sigma Hu_{intro} + f_I S^I$$

9. From the differences between the theoretical and the experimental integral data, use the fitting procedures to attempt to identify the errors created in step 5. These errors of cross sections are the differences between the theoretical and the true cross sections.

10. Interpret the result from the fitting procedures to make an evaluation of how effective the fitting procedures are; that is, how well the introduced cross section errors are identified.

Generation of Group Dependent Cross Sections

Since this study is to investigate the influence of the energy groups in data fitting, energy dependence of microscopic cross sections must be taken into consideration.

For the model used in this study, the definition of an averaged cross section $\bar{\sigma}$ is given by

$$\bar{\sigma} = \frac{\int_{E_L}^{E_U} \sigma(E)\varphi(E)\, dE}{\int_{E_L}^{E_U} \varphi(E)\, dE}$$

where E_L is the lower energy limit for the group defined, and

E_U is the upper energy limit for the group defined.

From this expression it is obvious that to obtain a group collapsed microscopic cross section for every isotope in an assembly one finds it necessary to perform a spectrum calculation; the multigroup diffusion code MACH-1[32] was used for this purpose. Since this study considers energy dependence up to four groups, the problem is to determine appropriate group boundaries of 2, 3, and 4 collapsed groups from the cross section library used which is the well known 26 group ABBN set.[31] To accomplish this, one can study the spectrum of Assembly 17, whose spectrum is typical of all the assemblies and was thus used in the previous one group study[22] to evaluate the one group collapsed cross sections. The group boundaries for this study were picked by decomposing the spectrum such that each collapsed group contains an almost equal amount of total fissioning rates. The 2, 3, and 4 group boundaries and their corresponding MACH-1[32] group boundaries are depicted in Tables 2, 3, 4, and 5.

For each choice of 2, 3, and 4 group cases, MACH-1[32] is used to perform a spectrum calculation for each assembly and then a calculation of group collapsing for each isotope in the assembly. The result is the group collapsed cross section set which may be regarded as the true values for this study.

Table 2. ABBN[31] Group Boundaries

Group	Range			
1	6.5	-	10.5	MeV
2	4.0	-	6.5	MeV
3	2.5	-	4.0	MeV
4	1.4	-	2.5	MeV
5	0.8	-	1.4	MeV
6	0.4	-	0.8	MeV
7	0.2	-	0.4	MeV
8	0.1	-	0.2	MeV
9	46.5	-	100	keV
10	21.5	-	46.5	keV
11	10	-	21.5	keV
12	4.65	-	10	keV
13	2.15	-	4.65	keV
14	1.0	-	2.15	keV
15	465	-	1000	eV
16	215	-	465	eV
17	100	-	215	eV
18	46.5	-	100	eV
19	21.5	-	46.5	eV
20	10.0	-	21.5	eV
21	4.65	-	10.0	eV
22	2.15	-	4.65	eV
23	1.0	-	2.15	eV
24	.465	-	1.0	eV
25	.215	-	.465	eV
26	.0252	-	.215	eV

Table 3. 2 Group Boundaries

Group	Range
1	.2 - 10.5 MeV
2	.0252 eV - 0.2 MeV

Table 4. 3 Group Boundaries

Group	Range
1	0.8 - 10.5 MeV
2	10 keV - 0.8 MeV
3	.0252 eV - 10 keV

Table 5. 4 Group Boundaries

Group	Range
1	1.4 - 10.5 MeV
2	0.2 - 1.4 MeV
3	4.65 keV - 0.2 MeV
4	.0252 eV - 4.65 keV

Fundamental Mode Analysis[29]

In order to study the effect of energy dependence on data fitting, this study has incorporated group structure in the cross section sets. However, the original assumption of the space independent diffusion theory in the previous one group study[22] remains unchanged. Assuming only one region and that the extrapolation distances are equal in all groups, the shape of the flux in every group can be represented by a common buckling term, that is, the fundamental mode. Then, one can evaluate the group dependent flux for a critical assembly by an iterative method.

The appropriate multigroup diffusion equation is

$$D_j \nabla^2 \phi_j - \Sigma_{a_j} \phi_j - \sum_{k=j+1}^{n} \Sigma_{j\to k} \phi_j + \sum_{k=1}^{j-1} \Sigma_{k\to j} \phi_k + \chi_j S_{f_o} = 0 \qquad (20)$$

where the fission source term is

$$S_{f_o} = \frac{\sum_{j=1}^{n} (\nu\Sigma_f)_j \phi_j}{k_{eff}} \qquad (21)$$

The equation relating to the fundamental assumption can be expressed by

$$\nabla^2 \phi_j(r) + B^2 \phi_j(r) = 0 \qquad (22)$$

Initially assuming a value for B^2 and unity for the fission source S_{f_o}, one can find φ_1 by substituting (22) into (20) and derive

$$\varphi_1 = \frac{\chi_1 S_{f_0}}{D_1 B^2 + \Sigma a_1 + \sum_{k=2}^{n} \Sigma_{1\to k}}$$

Similarly one can solve φ_2 in terms of φ_1 by substituting (22) into (20) and obtain

$$\varphi_2 = \frac{\chi_2 S_{f_0} + \Sigma_{1\to 2} \phi_1}{D_2 B^2 + \Sigma a_2 + \sum_{k=3}^{n} \Sigma_{2\to k}}$$

In general for any group j, φ_j can be expressed by

$$\varphi_j = \frac{\chi_j S_{f_0} + \sum_{k=1}^{j-1} \Sigma_{k\to j} \phi_k}{D_j B^2 + \Sigma a_j + \sum_{k=j+1}^{n} \Sigma_{j\to k}} \qquad (23)$$

Substituting the flux for every group into (21), one can calculate k_{eff}. In case k_{eff} is not equal to 1, one has to make another guess for B^2, recalculate the flux, and recheck the value of k_{eff} until the criticality is met.

Sensitivity Coefficients of Reaction Rate Ratios

If one substitutes the cross section functions, f_1 and f_2, by the known cross sections, σ_1 and σ_2, in the expression for the reaction rate ratio R specified in (18), one can express R in the form of

$$R = \frac{\int\int \sigma_1(E)\phi(r,E)\,dr\,dE}{\int\int \sigma_2(E)\phi(r,E)\,dr\,dE} = \frac{I_1}{I_2}$$

Eliminating the spatial dependence by use of the buckling approximation, the integrals in the numerator and the denominator can be reduced into summation over all groups.

$$R = \frac{\sum_i^n \sigma_{1,i}\phi_i}{\sum_i^n \sigma_{2,i}\phi_i}$$

where $\sigma_{1,i}$ stands for the averaged cross section of σ_1 in group i.

The calculation of the sensitivity coefficients for the reaction rate ratios used in this study is also dependent on the assumption of the fundamental mode analysis of a bare, homogeneous core. The calculation of flux is the same as described in (23).

Using the space independent, fundamental mode assumption, the iterative calculation of ψ_i^* in (19) can be avoided[33]; the problem is reduced to solving an equation similar to the diffusion equation used in the k calculation except that there is no fission source but a fixed source of the form:

$$S_i^+ = \frac{\sigma_{1,i}}{\sum_i^n \sigma_{1,i}\phi_i} - \frac{\sigma_{2,i}}{\sum_i^n \sigma_{2,i}\phi_i}$$

In addition, one has to evaluate the importance functions ψ_i^+ which can be considered as the importance of neutrons shown by the change of the reaction rate ratio due to the unit change of the φ_i at that energy. This is analogous to the definition of the normal adjoint function, φ_i^+.

The system of linear equations derived from the generalized perturbation theory to solve the importance functions ψ_i^+ is

$$-D_j B^2 \psi_j^+ - \Sigma_{a_j} \psi_j^+ - \sum_{k=j+1}^{n} \Sigma_{j\to k} \psi_j^+ + \sum_{k=j+1}^{n} \Sigma_{j\to k} \psi_k^+ + S_j^+ = 0 \qquad (24)$$

for $j = 1,2,\ldots,n$

where S_j^+ is the fixed source.

When the critical buckling B^2 is found, it can be substituted into (24) to solve for ψ_n^+, ψ_{n-1}^+, . . ., ψ_1^+ successively.

The expressions for ψ_n^+, ψ_{n-1}^+, and ψ_j^+ are

$$\psi_n^+ = \frac{S_n^+}{D_n B^2 + \Sigma_{a_n}}$$

$$\psi_{n-1}^+ = \frac{S_{n-1}^+ + \Sigma_{n-1\to n}\,\psi_n^+}{D_{n-1} B^2 + \Sigma_{a_{n-1}} + \Sigma_{n-1\to n}}$$

$$\psi_j^+ = \frac{S_j^+ + \sum_{k=j+1}^{n} \Sigma_{j\to k}\,\psi_k^+}{D_j B^2 + \Sigma_{a_j} + \sum_{k=j+1}^{n} \Sigma_{j\to k}}$$

The change of the reaction rate ratio R due to a change in nuclear cross section in the multigroup zero dimension model is

$$\frac{\delta R}{R}=\left[\sum_i \frac{\phi_i \delta\sigma_{1,i}}{I_1}-\sum_i \frac{\phi_i \delta\sigma_{2,i}}{I_2}\right]-\sum_i\left(\delta\Sigma_{a_i}+B^2\delta D_i\right)\phi_i\psi_i^+ +\sum_i\sum_j \delta\Sigma_{i\to j}\left(\psi_j^+-\psi_i^+\right)\phi_i+\sum_i \phi_i\,\delta(\nu\Sigma_f)_i \qquad (25)$$

The first combined term on the right of (25) is usually referred to as the direct effect, and the rest of the terms on the right are the spectral or indirect effect. As a final note one observes the expression for $\frac{\delta k}{k}$ can be obtained by substituting ψ_i^+ by φ_i^+ in the expression for $\frac{\delta R}{R}$, without the direct effect.

A study was performed by Salvatores[34] where results from the zero dimension fundamental mode calculation were compared with those from a one dimension diffusion code. The comparison showed the zero dimension fundamental mode analysis is adequate for the calculation of the sensitivity coefficients of the integral quantities at the core center of a large fast system.

Furthermore, for gedanken experiments, the sensitivity coefficients used to calculate the introduced cross section errors are the same as those used in the fitting. Thus the fundamental mode analysis is "exact" for this case.

Units of the Cross Section Error and the Sensitivity Coefficient

In the process of data fitting, one must select the proper units for the cross section error, so that the identified error can be reasonably applied to the established experimental differential data.

Since the true collapsed group cross section values in this study are different for every assembly, the most reasonable choice is to identify cross section error in percent; thus the identified error would either

raise or lower the group cross section value by the same percentage for all assemblies. This corresponds to maintaining the same differential cross section shape within the group for each assembly.

The self shielding effects are not considered in this study. However, various authors[9,15] have proposed methods of incorporating self shielding effects into the sensitivity coefficients.

Since the unit of introduced error is percent of the original cross section value, the corresponding sensitivity coefficient embodies the unit of per percent of cross section.

The transition of the unit of the sensitivity coefficient from per barn to per percent can be easily derived as follows.

Define H to be the sensitivity coefficient in units of per barn.

H' to be the sensitivity coefficient in units of per percent.

$\Delta\sigma$ to be some cross section change in barns.

x to be the same amount of cross section change in percent.

From the above definitions, one observes that

$$\Delta\sigma = \frac{x\,\sigma}{100} \tag{26}$$

Since the perturbation to the system, $\frac{\delta I}{I}$, is the same in both systems of different units, one obtains

$$H\,\Delta\sigma = H'x \tag{27}$$

Substituting (26) into (27), one concludes

$$H' = \frac{H\sigma}{100}$$

Sensitivity Coefficient of Cross Section Correlation Ratio

There are various types of cross section correlation. In this study, only the cross section correlation ratios are considered.

The sensitivity coefficient of cross sections can be transformed with ease to that of cross section correlation ratios, α, which are defined by

$$\alpha = \frac{\sigma_1}{\sigma_2} \tag{28}$$

In order to change the sensitivity coefficients of σ_1 and σ_2 into those of α and σ_2, one can use the following definitions:

Let H_1 be the sensitivity coefficient in units of per barn relating to $\Delta\sigma_1$,

H_2 be the sensitivity coefficient in units of per barn relating to $\Delta\sigma_2$,

and H_α be the sensitivity coefficient in units of per α relating to $\Delta\alpha$.

Thus the response of a critical system, $\frac{\delta I}{I}$, to a change in σ_1 and σ_2 can be expressed by

$$\frac{\delta I}{I} = H_1 \Delta\sigma_1 + H_2 \Delta\sigma_2 \tag{29}$$

Substituting (28) into (29), one obtains

$$\frac{\delta I}{I} = H_1 \Delta(\alpha\sigma_2) + H_2 \Delta\sigma_2$$

This can be simplified into

$$\frac{\delta I}{I} = H_1 \sigma_2 \Delta\alpha + (H_1\alpha + H_2)\Delta\sigma_2 \tag{30}$$

Since all the sensitivity coefficients are defined in units of per absolute magnitude, one has to transform them into units of per percent. One proceeds by proposing some more definitions:

Let x_α be the percent change equivalent to $\Delta\alpha$,

x_{σ_2} be the percent change equivalent to $\Delta\sigma_2$,

H_α be the sensitivity coefficient in units of percent of α,

and H_2' be the sensitivity coefficient in units of percent of σ_2,

Thus one readily states

$$\frac{\delta I}{I} = H_\alpha x_\alpha + H_2' x_{\sigma_2}$$

Knowing that the perturbation, $\frac{\delta I}{I}$, to a system is the same for either unit of the sensitivity coefficient, one observes that

$$H_\alpha x_\alpha = H_1 \sigma_2 \Delta\alpha \tag{31}$$

and

$$(H_1\alpha + H_2)\Delta\sigma_2 = H_2' x_{\sigma_2}$$

Using the relation between x_α and $\Delta\alpha$, (31) can be reduced to

$$H_\alpha = \frac{H_1 \sigma_2 \alpha}{100}$$

With the definition of α it can be further reduced to

$$H_\alpha = \frac{H_1\sigma_1}{100}$$

Similarly, the expression for H_2' would be

$$H_2' = \frac{H_1\sigma_1 + H_2\sigma_2}{100}$$

In conclusion one arrives at the obvious result that the sensitivity coefficient of α in per percent of α is identical to that of σ_1 in per percent of σ_1 whereas the sensitivity coefficient of σ_2 is identical to the sum of the sensitivity coefficients of σ_1 and σ_2 both in the units of per percent. This is physically reasonable considering the fact that a change in α with σ_2 holding constant is equivalent to a change in σ_1 whereas a change in σ_2 with α invariant is bound to induce a change in both σ_2 and σ_1 at the same time.

Errors of Differential and Integral Data

Cross Section Error

The estimated cross section uncertainties are produced from a survey[1,2,5,13] of various recent reliable sources of established information. Then the standard deviations of cross sections are extracted from the comparison between the cross section data. In general the standard deviations thus obtained represent a realistic survey on the present accuracy of nuclear data.

The standard deviations of cross sections for 2, 3, and 4 groups are given in Tables 6, 7, and 8.

Table 6. Standard Deviations of 2 Group Cross Sections

	σ_{c_1}	σ_{f_1}	σ_{tr_1}	σ_{c_2}	σ_{f_2}	σ_{tr_2}
Pu-239	5	3	20	5	3	10
Pu-240	10	3	20	10	3	20
U-235	5	3	20	5	3	10
U-238	10	3	20	10		10
Fe	20		20	15		15
Ni	20		10	15		10
Cr	25		15	20		10

Table 7. Standard Deviations of 3 Group Cross Sections

	σ_{c_1}	σ_{f_1}	σ_{tr_1}	σ_{c_2}	σ_{f_2}	σ_{tr_2}	σ_{c_3}	σ_{f_3}	σ_{tr_3}
Pu-239	5	3	20	5	3	15	5	5	10
Pu-240	10	3	20	10	3	20	10	3	20
U-235	5	3	20	5	3	15	5	3	10
U-238	10	3	20	10		20	10		20
Fe	20		20	20		20	10		10
Ni	20		10	20		10	10		10
Cr	20		20	25		10	10		5

Table 8. Standard Deviations of 4 Group Cross Sections

	σ_{c_1}	σ_{f_1}	σ_{tr_1}	σ_{c_2}	σ_{f_2}	σ_{tr_2}	σ_{c_3}	σ_{f_3}	σ_{tr_3}	σ_{c_4}	σ_{f_4}	σ_{tr_4}
Pu-239	5	3	20	5	3	20	5	3	10	5	5	10
Pu-240	10	3	20	10	3	20	10	3	20	10		20
U-235	5	3	20	5	3	20	5	3	10	5	3	10
U-238	10	3	20	10	3	20	10		10	10		10
Fe	20		20	20		20	20		20	5		10
Ni	20		10	20		10	20		10	10		10
Cr	20		20	25		10	25		10	7		5

Criticality Factor Error

The criticality factor error can contribute to the difference between the calculated and the measured k values. Moreover, this error can be specifically divided into statistical and systematic errors.

The statistical errors are mainly due to inevitable errors in carrying out the experimentation, such as the measurement of counting rates, atom concentrations, etc. The systematic errors are due to intrinsic errors in methods of calculation, the assumptions and models of the methods applied, and experimentation. In particular, heterogeneity corrections and shape factor adjustments for one dimensional non-spherical models constitute a major portion of the error whereas the corrections for irregular boundaries, discrepancies in the measured critical mass possibly from non-uniform fabrication of the fuel elements, yield a minor part of the criticality factor error.

In most cases of this study, the standard deviation S^I for the experimental errors of the reactivity was varied from 0.1% up to 0.5% for a realistic representation.[35] The systematic error of the reactivity was varied from -2% to 2% in studies of the influence of systematic errors in particular.

Reaction Rate Ratio Error

The standard deviations for the error in the experimental reaction rate ratio are in the order of a few percent, which is considerably larger than that of k values.

The sources of experimental errors may be attributed to improper calibration of fission chamber, interference of the high gamma background, various errors in activation analysis, etc.

The standard deviation S^I for the experimental error of reaction rate ratio was varied from 3% to 7%[36] in this study. Furthermore, the systematic error of the reaction rate ratio was varied from -0.2 to 0.2 in studies of the influence of this type of error in particular.

Cross Section Correlation Error

From the standard deviation of all the cross sections, it is obvious that the capture cross section of a heavy fissile element has a much larger uncertainty than that of the fission cross section. Due to the difficulty of a direct measurement of the capture cross section, one generally measures the ratio of a capture cross section with respect to the fission cross section of some standard isotopes such as U-235; furthermore, ratios of the fission cross section of one isotope to that of the standard isotope are also measured to determine the fission cross section of the numerator isotope. A list of conspicuous examples is the capture of U-238 to the fission of U-235, the fission of U-238 to the fission of U-235, and the fission of Pu-239 to the fission of U-235

As more experimenters obtain higher accuracy of the measurements of reaction rate ratios, the idea of using these ratios in fitting procedures to seek information on the cross sections which are hard to measure is well justified.

In this study not only correlations between different isotopes are incorporated, but correlations between various cross section types in the same isotope are also considered, for example, capture of U-235 to fission of U-235, and capture of Pu-239 to fission of Pu-239.

The errors of various correlation types[37] are shown in Tables 9 and 10.

Table 9. Estimated Standard Deviations of Cross Section Correlation Ratio Between Different Isotopes

Groups \ Pu-239 / U-235	$\frac{\sigma_{c_1}}{\sigma_{f_1}}$	$\frac{\sigma_{f_1}}{\sigma_{f_1}}$	$\frac{\sigma_{c_2}}{\sigma_{f_2}}$	$\frac{\sigma_{f_2}}{\sigma_{f_2}}$	$\frac{\sigma_{c_3}}{\sigma_{f_3}}$	$\frac{\sigma_{f_3}}{\sigma_{f_3}}$	$\frac{\sigma_{c_4}}{\sigma_{f_4}}$	$\frac{\sigma_{f_4}}{\sigma_{f_4}}$
2	4	3	4	3				
3	4	3	4	3	4	4		
4	4	3	4	3	4	3	4	4
U-238 / U-235								
2	5	3	5					
3	5	3	5		5			
4	5	3	5	3	5		5	
Pu-240 / Pu-239								
2	4	3	4	3				
3	4	3	4	3	4	3		
4	4	3	4	3	4	3	3	
U-238 / Pu-239								
2	5	3	5					
3	5	3	5		5			
4	5	3	5	3	5		3	

Table 10. Standard Deviation of the Cross Section Correlation Ratio Within the Same Material

Groups \ U-235/U-235	$\frac{\sigma_{c_1}}{\sigma_{f_1}}$	$\frac{\sigma_{c_2}}{\sigma_{f_2}}$	$\frac{\sigma_{c_3}}{\sigma_{f_3}}$	$\frac{\sigma_{c_4}}{\sigma_{f_4}}$
2	4	4		
3	4	4	4	
4	4	4	4	4
Pu-239/Pu-239				
2	4	4		
3	4	4	4	
4	4	4	4	4

Sampling of Fractional Values of Errors

Since the outcome of a meaningful solution from the fitting procedures depends crucially on the randomness of the errors selected in both the cross sections and the experimental integral data, a rigorous attempt was made to sample the fractional values from a standard Gaussian distribution. However, instead of sampling from the distribution, one can use an easier approach via the uniform distribution and obtain good statistics as well. The method is described in Appendix B. The uniform distribution routine is obtainable from the UNIVAC Mathpack.[38]

CHAPTER IV

COMPUTER PROGRAMMING SCHEDULES

Storage Allocation and Nomenclature

The versatile computing system at Georgia Tech is a UNIVAC 1108 which has a 196 K words core and more than 40 million words of mass storage on the Fastrand system.

To allocate storage on Fastrand one must first assign a file. Because of the administration of files on Fastrand, the optimum usage of this facility pressures the user to keep his files as few as possible in order that they may be reassigned more readily. Consequently, considerable work in this dissertation involves developing the most effective means of data allocation.

The general nomenclature for a data or program element ELEMENTB in a file FILEA will be denoted in consistence with UNIVAC Exec System[39] as "FILEA.ELEMENTB". This notation will be adopted throughout the entire study.

Creating the Cross Section Files

One of the unique differences of this study from the previous one group study is the consideration of the energy dependence, ranging from 2 to 4 groups.

To evaluate the group dependent, spectrum averaged cross section for each isotope in each of the 50 assemblies used in this study, one needs to first perform a spectrum calculation for every composition and then group

collapse for each isotope in that composition, as previously described.

The one dimensional diffusion code MACH-1,[32] with the handy option of punching out the collapsed microscopic cross sections in cards, was used to execute these operations. Thus, with three choices of energy groups and 50 assemblies, at least 150 MACH-1[32] runs are required. Even though performing these runs is routine, the preparation of input data to these runs requires meticulous care and is inevitably time consuming. To avoid any possible error, a program RED.PUNCH was written to punch out the number density of every isotope in any assembly in the format acceptable to the MACH-1[32] input.

The punched cross section images from MACH-1[32] were stored on DATE.SIG2, DATE.SIG3, and DATE.SIG4 where the digits 2, 3, and 4 refer to numbers of energy groups.

The program DATE.LIST was then executed using these three elements in DATE and some other input description to create the cross section file for each different group. The names of cross section files are CROSS2, CROSS3, CROSS4 where the digits 2, 3, and 4 designate the number of energy groups.

Creating Data Elements of Sensitivity Coefficients for the Integral Data

A program RED.K was developed to calculate the flux, its adjoint, and the sensitivity coefficients for k. The perturbation expressions were derived from the classical theory.

After this program was tested successfully, it was copied into RED.RR where the calculation of flux and its adjoint remains intact but

many changes were incorporated to evaluate the sensitivity coefficients for reaction rate ratios based on the generalized perturbation theory, as described in (25).

Both these programs required cross section files and option description as input to generate the related sensitivity coefficients on data files assigned temporarily.

Then the temporary files together with group and format description were read in by RED.CONVERT to be converted into elements of ID. As a result, all the sensitivity coefficients for either k or reaction rate ratios are stored in elements of ID instead of individual data files. This eliminates the necessary waiting for data files in case they are not loaded in the core.

Test cases were run to check results of RED.K and RED.RR against those of CIAP-O[34] which is a zero dimensional multigroup generalized perturbation code. The consistent agreement in every case indicated there exists no error in RED.K and RED.RR.

Running Four Fitting Procedures Simultaneously

Since this study is based on statistics, a myriad of test cases consisting of minor adjustments of input parameters is involved. To expedite setting up the tedious input to the fitting programs, a program BLACK.KRR was established to read the sensitivity coefficients from elements of ID and other relevant input options to create a temporary data file which contained all the commands and the necessary input for executing the four fitting procedures. Then simply by adding the temporary data file into the core, a cascade of cases would be run.

The debugging of each fitting procedure constituted a considerable effort. In order to eliminate any error due to adding options to the programs, each program was built on a module concept; that is, every subroutine was individually debugged and tested before it was implemented into the main program. Since the four fitting procedures demanded similar forms of equations to solve, many subroutines were shared by all fitting procedures, which considerably facilitated the solutions.

The accuracy and the logic of the four fitting procedures were substantiated by checking against hand calculations for some simple cases, and against some previous results of Kallfelz's one group calculations.[22]

The following three flow charts (Figures 1, 2, and 3) depict what has been discussed.

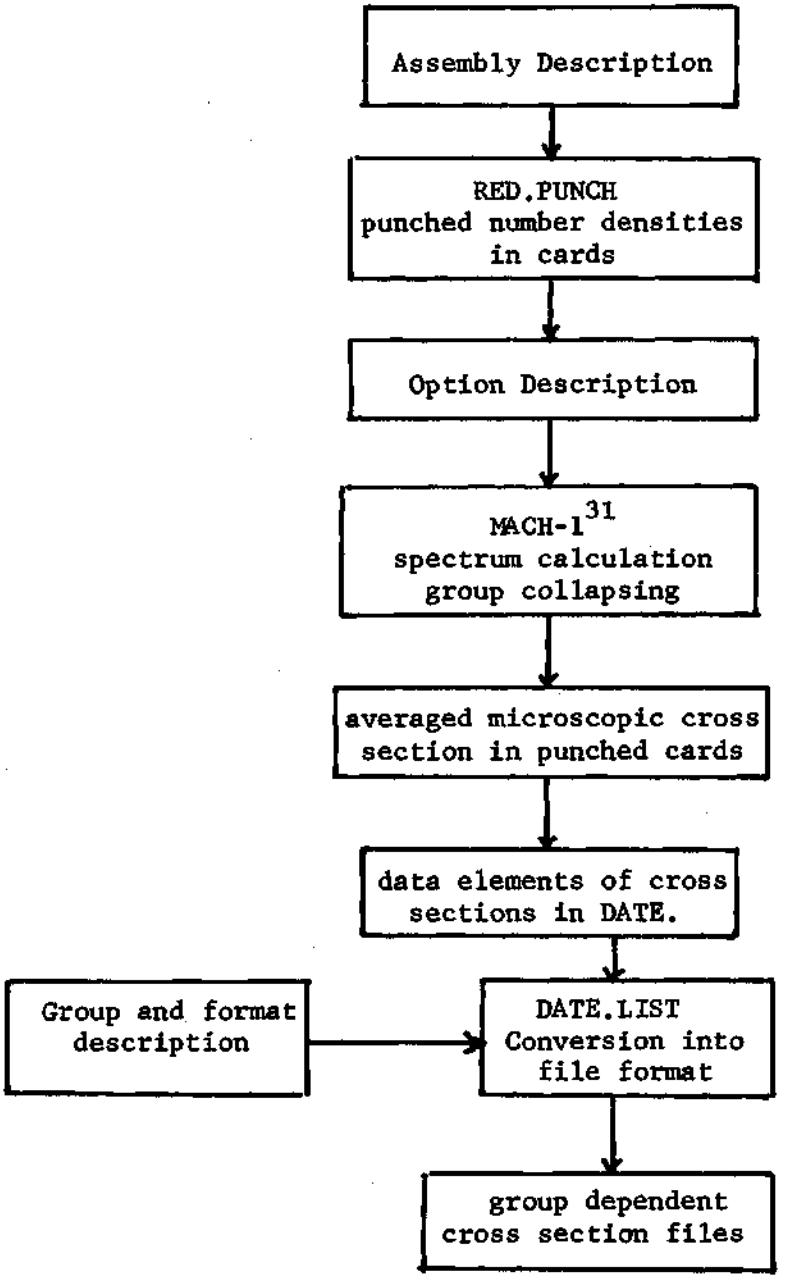


Figure 1. Creating the Cross Section Files

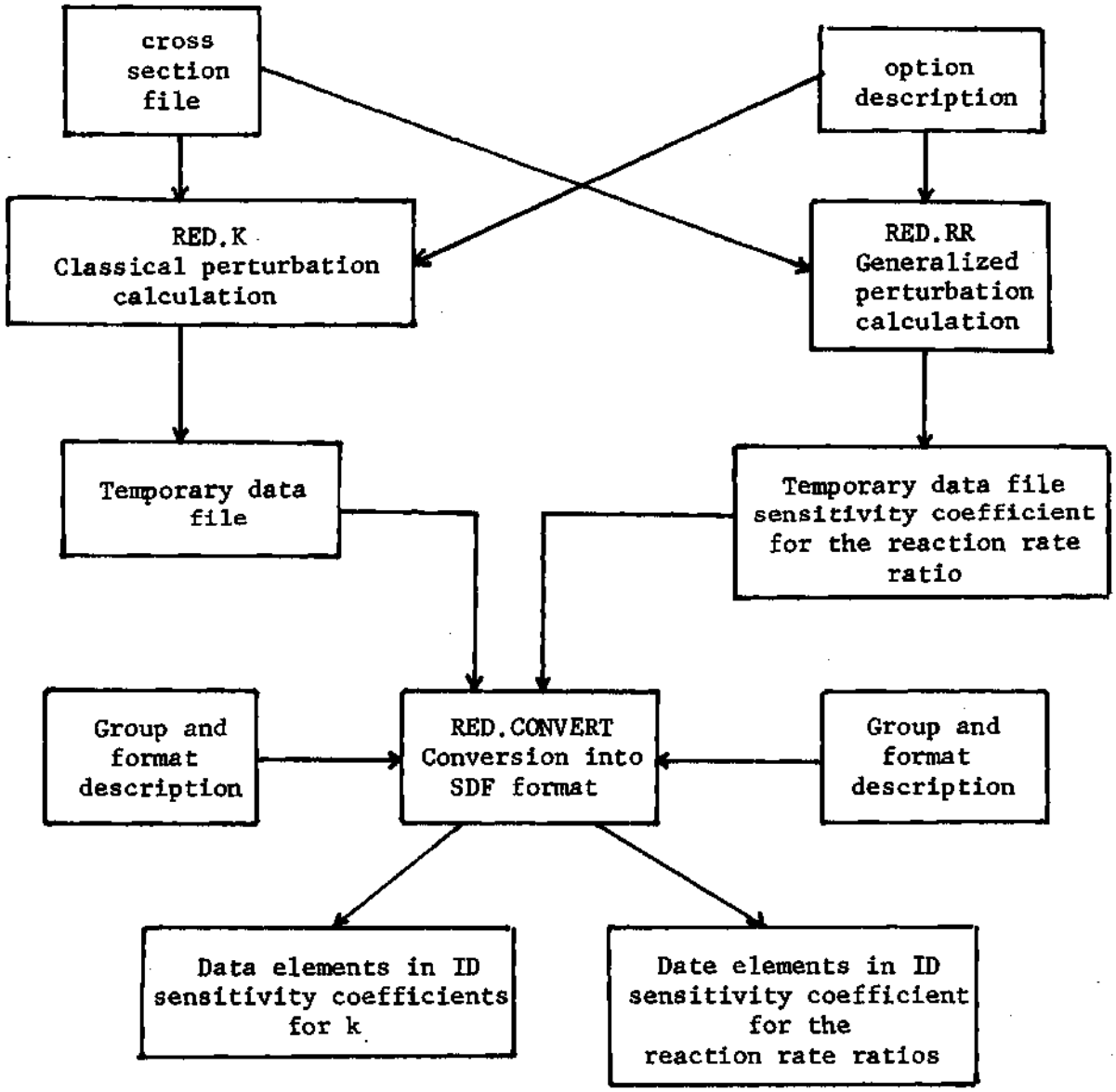


Figure 2. Creating Data Elements of Sensitivity Coefficients for the Integral Data

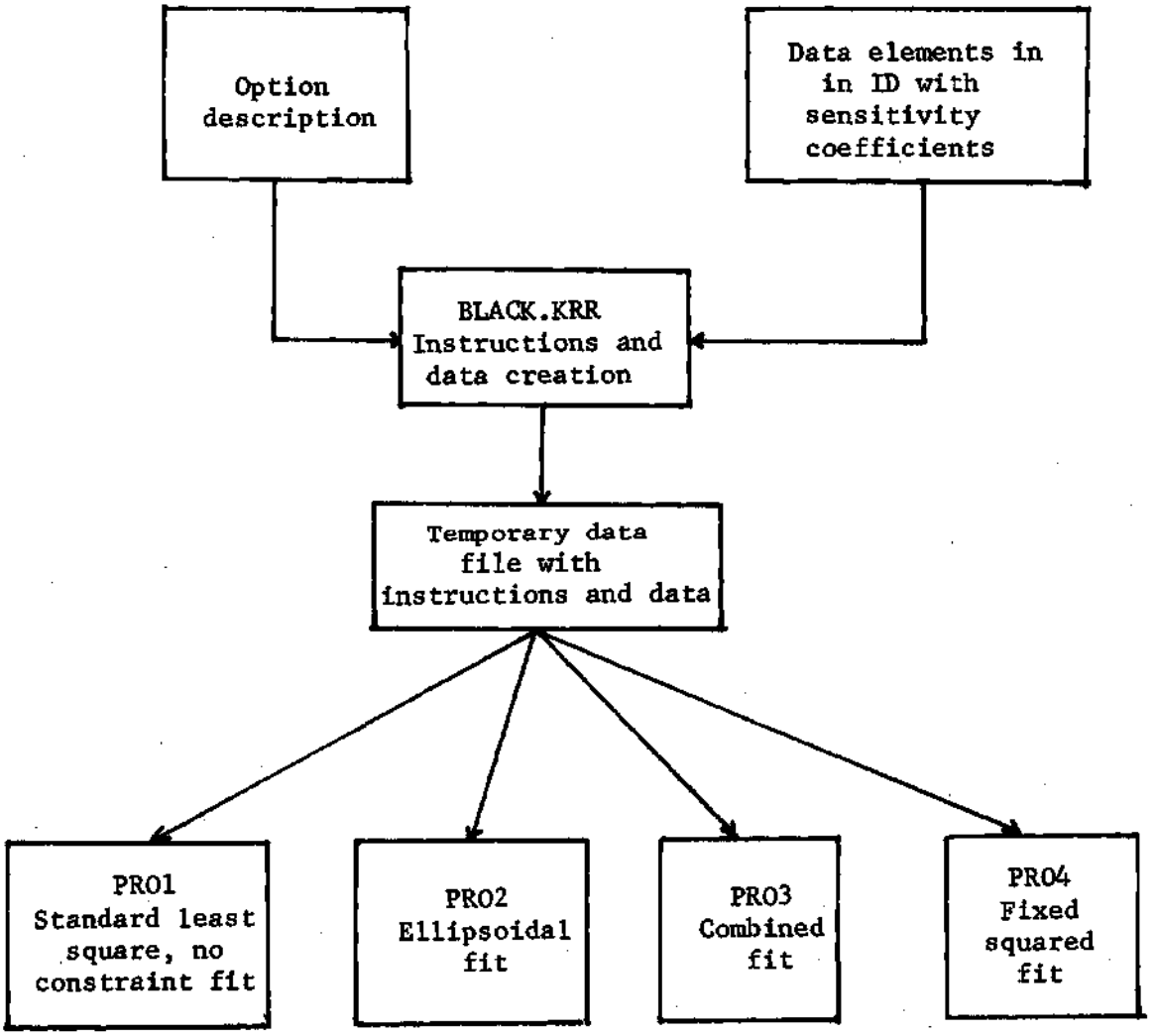


Figure 3. Running Four Fitting Procedures Simultaneously

CHAPTER V

RESULTS AND DISCUSSION

Description of Data Sets

The data sets which contain input to fitting procedures are readily saved in the data elements of the file BLACK.. The following is a tabulated description of all data elements in which the file name BLACK. is omitted for brevity (Table 11).

Comparison between Fitting Schemes

The choice of the "best" fitting scheme has aroused dispute among numerous groups. The four basic fitting procedures, namely the standard least square, no constraint fit, the ellipsoidal fit, the combined fit, and the fixed square fit, can be used to investigate the principal schemes being used or proposed in the past and the present.

The choice of the favorable schemes among the four listed may be based on two realistic criteria:

(1) The amount of information discovered by the fitting scheme

(2) The practical workability of the scheme.

With regard to criterion (1), the measure of the information which the fitting scheme reveals should be based on how well the scheme identifies the nuclear errors introduced in fitting.

In general one can define a figure of merit to indicate the percentage of the introduced errors the fitting scheme can reveal; thus a figure of merit should depend on the interrelationship between the two

Table 11. Description of Data Sets

Data Element	Groups	Unknowns	k	$\frac{\sigma_c^{238}}{\sigma_f^{235}}$	$\frac{\sigma_f^{238}}{\sigma_f^{235}}$	$\frac{\sigma_c^{238}}{\sigma_f^{239}}$	$\frac{\sigma_f^{238}}{\sigma_f^{239}}$	$\frac{\sigma_c^{240}}{\sigma_f^{239}}$	$\frac{\sigma_f^{240}}{\sigma_f^{239}}$	Assembly
.2D8T5-2G	2	10.		10	10					21 up to 30
.2D8T5-2G-FE	2	14		9	9					21 up to 30 except 28
.3D8T9-2G	2	10	10			10	10			1 up to 10
.3D8T9-2G-1	2	10	20			20	20			1 up to 20
.3D8T9-2G-2	2	10	40			40	40			1 up to 20 31 up to 50
.3D8T5-3G-FE	3	22	9	9	9					21 up to 30 except 28
.2D8T5-3G	3	16		10	10					21 up to 30 except 28
.2D8T9-3G	3	16				40	40			1 up to 20 31 up to 50
.DK09CF-3G-FE	3	24	9					9		31 up to 40 except 38
.2D0T9-3G-FE	3	24						9	9	31 up to 40 except 38
.DK09FF-4G	4	18	10						10	31 up to 40
.DK09CF-4G-FE	4	30	9						9	31 up to 40 except 38
.3D8T5-4G-FE	4	30	9	9	9					21 up to 30 except 28

variables, namely the introduced error and the identified error. In essence, the figure of merit is a parameter designed to give some true indication of the effectiveness of the error identification by a fitting scheme.

For the previous one group study,[22] the "old" figure of merit was defined to be

$$f\left(\frac{n}{2}\right) = \frac{\sum_{k=1}^{\frac{n}{2}} \left(\frac{1}{S_k^{\sigma}}\right) \left| u_{iden}^{k} - u_{true}^{k} \right|}{\sum_{k=1}^{\frac{n}{2}} \left(\frac{1}{S_k^{\sigma}}\right) \left| u_{true}^{k} \right|}$$

where

u_{iden}^{k} is the error of cross section identified by fitting

u_{true}^{k} is the true error of that cross section

S_k^{σ} is the standard deviation of the cross section

n is the total number of nuclear cross section errors

k is the index for any one of the best conditioned 50% of the unknowns.

The "best conditioned" 50% of the unknowns u^k originated from a terminology of "ill conditioned variable" introduced by Ott.[22] If the standard deviation of the identified error, S_k^u, of the cross section is greater than that of the cross section, S_k^{σ}, then clearly the identified error is of limited use. Therefore, one appropriate definition of an "ill conditioned" variable is any variable which satisfies the condition that

$$r_k \equiv \frac{S_k^u}{S_k^{\sigma}} \geq 1$$

where S_k^u is the estimated standard deviation of the identified error u_{iden}^k, and

S_k^σ is the standard deviation of the cross section.

One can calculate the complete set of ratios r_k; by arranging the set of r_k in increasing order, one can declare that the unknowns corresponding to the first half of the arranged set of r_k are the best conditioned 50% of unknowns.

From the definition of the "old" figure of merit, if there exist many small introduced errors, which will often result in small identified errors after fitting, they might cause a relatively large figure of merit, since for small introduced errors the identified errors might also be small, but considerably different in absolute value (or even of opposite sign) than the introduced errors. Thus the figure of merit tends to be unfair to the small introduced errors.

In the previous one group study,[22] all fractional values of cross section errors were obtained by random coin flipping. Although these fractional values are adequate for the rough approximation of a Gaussian distribution, they are often larger than those encountered in this study which utilizes a more sophisticated simulation of a Gaussian distribution. Consequently, most errors introduced for the important cross sections in the previous one group study[22] were so large that one did not notice the unfair biasedness of the "old" figure of merit toward the small introduced error.

In this study the "new" figure of merit is the average of all the individual figures of merit of cross section errors. The following is a detailed description of the definition of the figure of merit of individual

cross section error.

(1) If the introduced error is relatively large, that is, if $|u^k_{intro}| \geq 0.1\ S^\sigma_k$, then check to see if the identified error, u^k_{iden}, satisfies the following two rules:

(a) The identified error, u^k_{iden}, must have the same sign as the introduced error, u^k_{intro}.

(b) If

$$\left| \frac{u^k_{iden}}{u^k_{intro}} \right| \leq 2.0$$

then one calculates the figure of merit of cross section k as

$$(f.m)_k = \left| \frac{u^k_{iden} - u^k_{intro}}{u^k_{intro}} \right|$$

For any u^k_{iden} which does not satisfy these two rules, one automatically assumes its $(f.m)_k = 1.0$.

(2) If the introduced error is relatively small, that is, if $|u^k_{intro}| \leq 0.1\ S^\sigma_k$, check to see if $||u^k_{iden}| - |u^k_{intro}|| \leq 0.1\ S^\sigma_k$.

Finally the overall "new" figure of merit of all the cross section errors is calculated by

$$F.M. = \frac{1}{n} \left[\sum_{k=1}^{n} (f.m)_k \right]$$

The rules for this definition of $(f.m)_k$ are based on intuitive reasoning:

The rule (1a) checks that the error identified with initially intro-

duced large error has the same sign as the introduced value.

The rule (1b) prevents the $(f.m)_k$ from being larger than 1.0 which is by this definition the worst error identification one can get. By restricting $(f.m)_k$ to a value not more than 1.0, one does not allow the ill conditioned variables to offset the other variables. This reasoning is similar to that used in the one group study[22] which deletes the 50% of the variables in the calculation of the "old" figure of merit.

The rule (2) states, if the introduced error is significantly small and the error identified is also quite small compared with S_k^σ, then the fitting scheme has obviously done a good job in identifying a small error and should be rewarded accordingly.

Theoretically speaking, the lowest or the most optimistic value of the "new" figure of merit can be 0.0, which infers that the introduced error and the identified error are either equal or both quite small compared with S_k^σ.

As a final note on the definition of the "new" figure of merit, one notices that it is an average of all the individual figures of merit. This expression stems from the fact that the overall figure of merit should represent on the average the fraction of the introduced errors that the data fitting identifies.

The four fitting adjustment procedures can be compared through the use of a parameter, β, in the ellipsoidal constraint procedure. The previous one group study[22] has extensively adopted this parameter in the comparison of results from fitting schemes.

The definition of β is given by

$$\omega_k = \beta s_k^{\sigma} \tag{32}$$

where w_k is the axis of the constraint ellipsoid.

Recall that the equation for the ellipsoid is

$$\sum_k \frac{u_k^2}{\omega_k^2} = 1 \tag{33}$$

Substituting (32) into (33), one obtains a simple expression for an equivalent beta, once the identified errors u_k have been determined. That is,

$$\beta = \left[\sum_k \frac{u_k^2}{(s_k^{\sigma})^2} \right]^{\frac{1}{2}}$$

Since different fitting schemes will give different beta values and different figures of merit after fittings, one can compare these fitting schemes by plotting their figures of merit versus betas on the same curve.

In the previous one group study,[22] the "old" figure of merit versus beta curve is usually an upside down bell shape; that is, as the beta increases from 0, the "old" figure of merit decreases from a value of 1.0 to a minimum and then increases until it reaches a plateau beyond which there is no further change of curve. At the point where no constraint on the cross section errors applies, the curve stops.

In this study, which involves 2, 3, and 4 group dependence, the "new" figure of merit versus beta curve frequently retains a similar shape.

As shown in Figure 4 for a typical case, as beta increases from 0, the "new" figure of merit proceeds from a value of 1.0, which implies no identification of any error, down to a minimum (0.56 in this case, which is an indication of good error identification). As the beta increases farther, the error identification starts to deteriorate.

The shape of this curve can be explained by first studying the behavior of the curve at the two extreme magnitudes of beta. At beta much less than 1, there is little variation allowed on the cross section; thus the error identified has to have small magnitude. As a result, not much information can be extracted from the fitting on the improvement of the nuclear data. In the most extreme case of $\beta = 0$, one observes the errors identified are zero. For the other extreme case, as the beta increases without bound, the nuclear uncertainties can vary in such large dimensions that the ellipsoidal fit becomes the standard least square, no constraint fit. Increasing beta beyond that point, the "new" figure of merit will not vary since the fitting remains the standard least square, no constraint case.

The second realistic criterion of selecting a fitting procedure is to determine how easily that procedure can be applied. In a practical situation where a large number of unknowns is involved, one has to resort to sophisticated computer techniques for the inversion of a large matrix. Hence from the consideration of the computer time, the combined fit, which does not require any iteration, is obviously more favorable than the ellipsoidal fit and the fixed square fit, each of which requires at least five iterations to determine the La Grange multiplier, that is more than five times the computer time needed for an equivalent combined fit case.

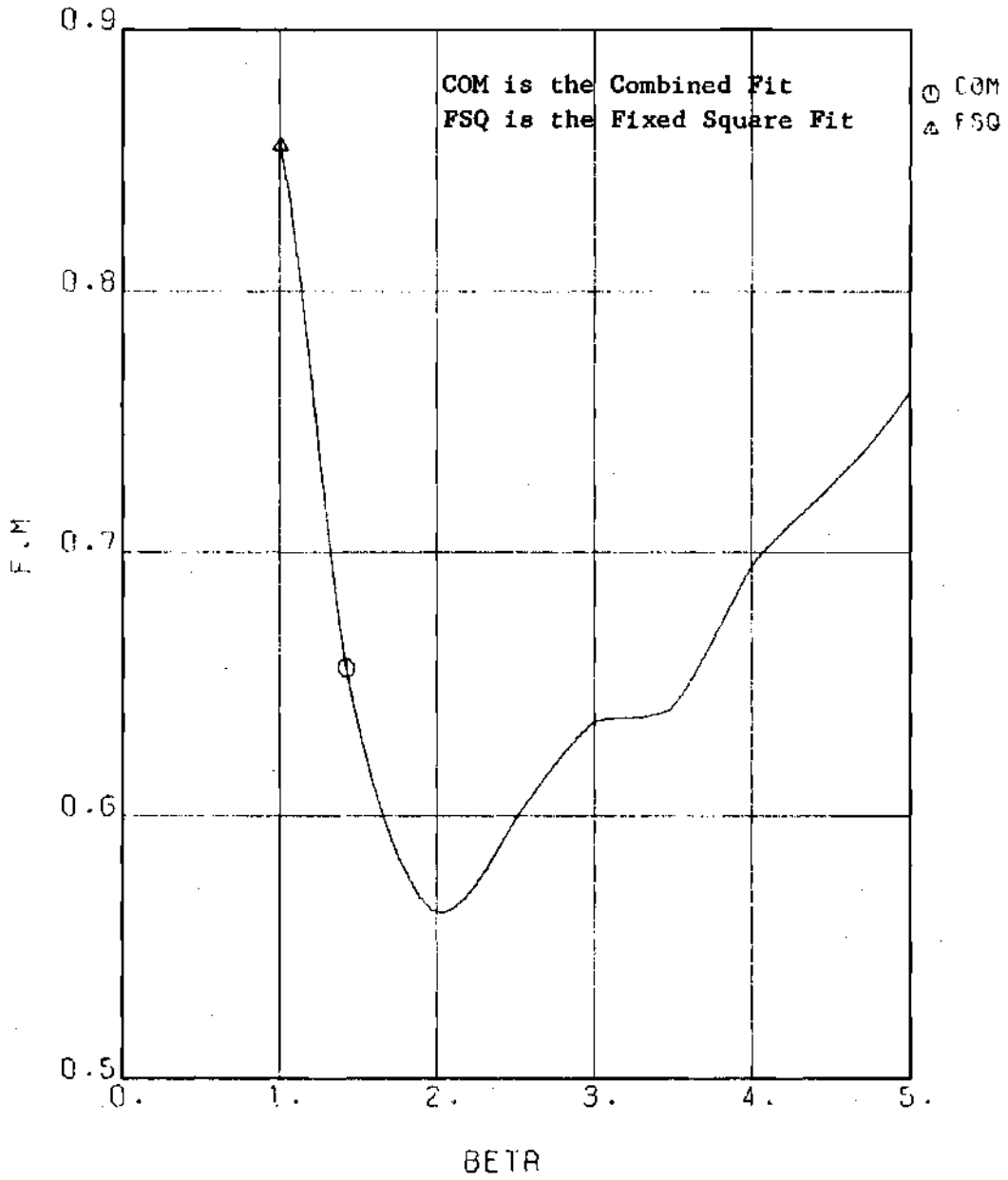


Figure 4. Figure of Merit versus Beta BLACK.3D8T5-3G-FE with 3 Groups, 22 Unknowns, 9 k Values with S^I = .001, 18 Reaction Rate Ratios with S^I = .03

From the numerous cases run, the standard least square, no constraint fit is proven to be highly ineffective when compared with the results of other fitting schemes. Though the result for the overdetermined case of the standard least square, no constraint fit obtained by fitting may minimize the square deviation between the theoretical and the experimental integral data, there is no constraint on the cross section whatsoever; one often finds that the identified errors deviate tremendously from the introduced errors unless the case is very overdetermined. As a rule the "new" figure of merit thus derived is in the neighborhood of 1.0, giving an indication of poor identification of errors.

From the underdetermined case of the standard least square fit, one can find a unique solution if one defines the problem (see p. 20) as finding, among the solutions that minimize the square deviation between the theoretical and the experimental integral data, the one which also minimizes the sum of squares of cross section changes. The results of many such cases show that the magnitude which the identified cross section errors deviate from the introduced values is generally larger than that encountered in the related overdetermined case. The trouble lies in the computation of the pseudoinverse of the matrix of sensitivity coefficients. As such a matrix does not have a full column rank, the round-off error in the computation is so large that one cannot avoid erroneous results. This can be explained by examining the theorem in the previous discussion

$$H^{+} = \lim_{\delta \to 0} (H^{T}H + \delta^{2}I)^{-1}H^{T}$$

As δ approaches zero, $(H^T H + \delta^2 I)$ is approaching $H^T H$ and getting more and more singular. At the condition $\delta = 0$ where the pseudoinverse exists, a slight variation of δ would produce a gigantic contribution of round-off error which may be definitely carried into the result. Thus one reaches the inevitable conclusion that, though for the underdetermined case of the standard least square fit the use of the model specified in the previous discussion mathematically gives a unique solution, the solution is not very helpful as far as the practical application is concerned. As the number of integral experiments increases, the error identification does not improve significantly as evidenced in many cases as long as the underdetermined condition is still kept.

In conclusion one believes the standard least square fit is not well equipped to meet the challenge of a multigroup data fitting.

Two Measures of Information

In addition to the figure of merit, there exist two parameters which were used in the previous one group study[22] as further measures of information obtained.

The first one defined in the previous one group study[22] is the average discrepancy between the experimental and the theoretical reactivity.

$$\overline{\Delta\rho(\beta)} = -\frac{1}{N}\sum_n \left[\rho_n^{ex} - \rho_n^{th} \right] \tag{34}$$

The second is the average square discrepancy between the experimental and the theoretical reactivity.

$$\overline{\Delta\rho^2(\beta)} = \frac{1}{N}\sum_n \left[\rho_n^{exp} - \rho_n^{th}\right]^2 \qquad (35)$$

Since in the one group study[22] the integral data employed were k values only, one expects that in the ideal case the two measures of information obtained after fitting would be proportional to the experimental errors of the k value. That is, $\overline{\Delta\rho(\beta)} = \frac{1}{\sqrt{N}} S^{\rho}$ for very large N

$$\sqrt{\overline{\Delta\rho^2(\beta)}} = S^{\rho}$$

If the two measures of information derived after fitting are much less than their experimental counterparts, for example, $\sqrt{\overline{\Delta\rho^2}} \ll S^{\rho}$, then the fitting is overdone.

In this study where both the reaction rate ratio and k are considered, the above expressions (34) and (35) do not apply since S^I is intended for one type of integral data only. To incorporate the effect of different S^I, the two measures of information are redefined as follows:

$$\Delta I(\beta) = -\frac{1}{N}\sum_n \left[\frac{I_n^{exp} - I_n^{th}(\beta)}{S^I}\right]$$

$$\overline{\Delta I^2(\beta)} = \frac{1}{N}\sum_n \left[\frac{I_n^{exp} - I_n^{th}(\beta)}{S^I}\right]^2$$

For $\beta = 0$, there is no identification, in other words, the corresponding ellipsoidal fit, which in this case yields no error identification, is confined by a zero constraint. Therefore, $\overline{\Delta I(o)}$ and $\overline{\Delta I^2(o)}$ in essence represent the errors before fitting. As beta increases from zero, the fitting schemes are gradually reducing the absolute magnitudes of these

two measures of information until they reach the values where the fixed square condition is met, there is $\overline{\Delta I^2} = 1.0$, and increasing beta much further will result in an overfit of data. Consequently, one observes in many cases as beta increases to its maximum, which corresponds to the standard least square, no constraint fit, the two measures of information thus obtained are smallest in absolute magnitude; nevertheless, the fitting is meaningless since the identified errors are much larger than the introduced errors, and the figure of merit is usually 1.0.

Sometimes as beta increases, the fitting may yield a larger $\overline{\Delta I}$ than the one for a smaller beta, because of the cancellation of individual ΔI values with opposite signs, even though the individual ΔI are generally getting smaller. At any rate, the general trend is that as beta increases, the absolute magnitude of $\overline{\Delta I}$ decreases. As for the $\overline{\Delta I^2}$, the trend is always decreasing as beta increases. The reasoning is twofold; the first reason is that $\overline{\Delta I^2}$ is related to the sum of the squares of all the individual average discrepancies between the experimental and the theoretical integral data, and is never negative; the second reason is that, as beta increases, more and more weight is put on minimizing ΔI^2 in the fit whereas the weight on the constraint for the cross section errors is less and less; hence ΔI^2 is decreasing. The behavior of $\overline{\Delta I}$ and $\overline{\Delta I^2}$ versus beta for one case is shown in Figures 5 and 6.

The Choice of Weighting Factor for the Combined Fit

There has been considerable discussion among various investigators concerning the optimal choice of the weighting factor between the integral and the differential terms in (3), for the combined fit (PRO3). While

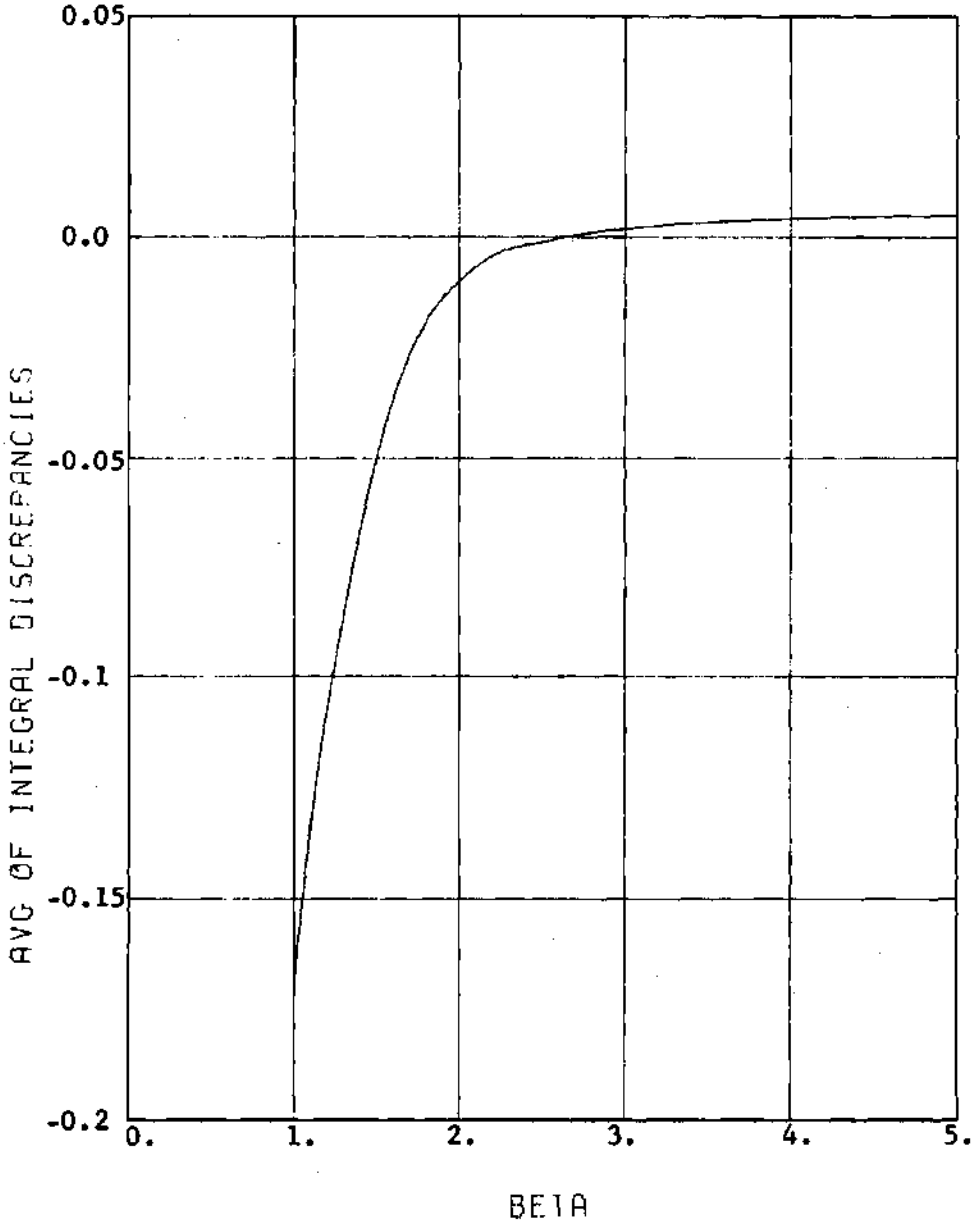


Figure 5. Average of Integral Discrepancies versus Beta BLACK.2D8T5-2G-FE with 2 Groups, 14 Unknowns, 18 Reaction Rate Ratios with S^I = .03

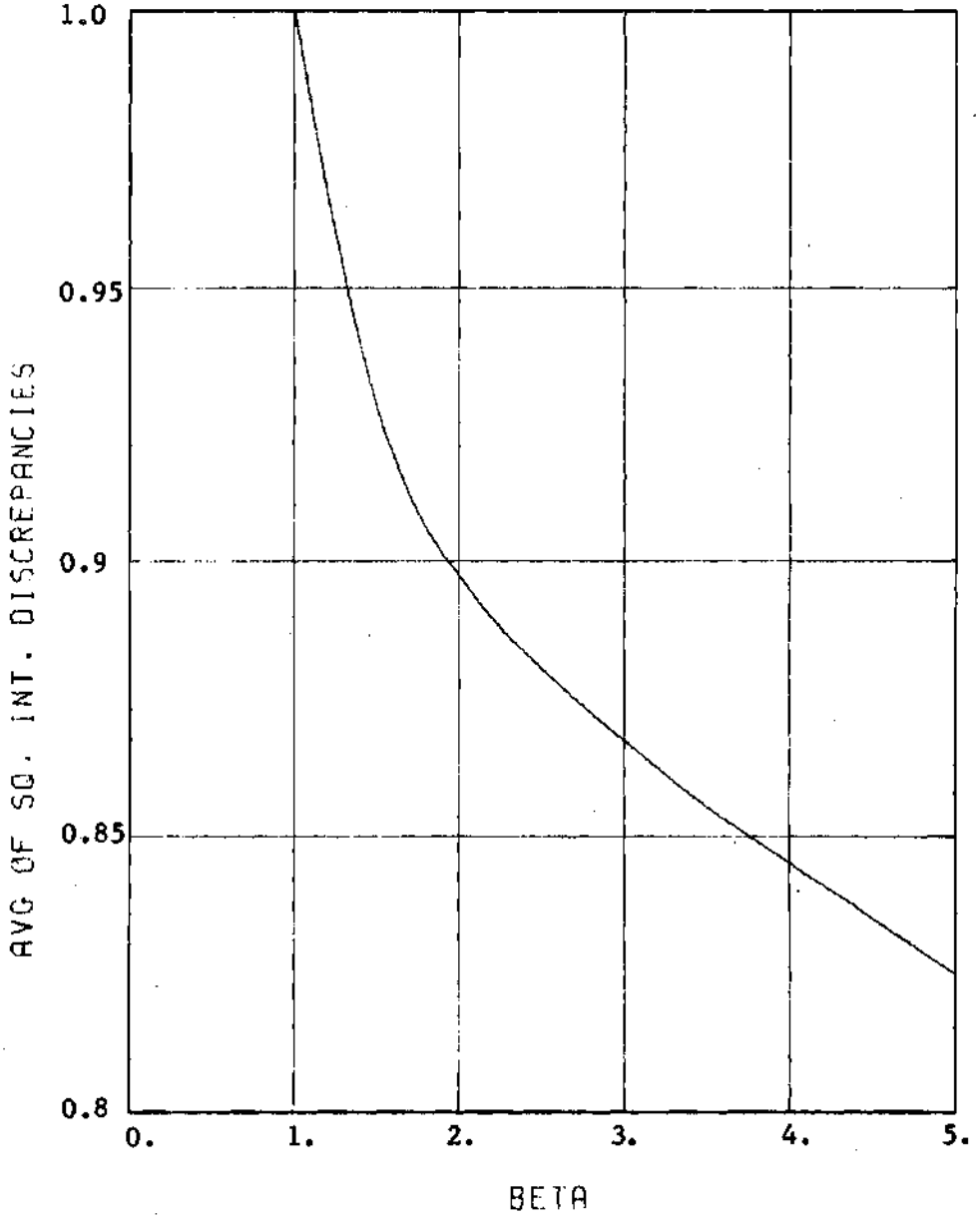


Figure 6. Average of the Square of the Integral Discrepancies versus Beta BLACK.2D8T5-2G-FE with 2 Groups, 14 Unknowns, 18 Reaction Rate Ratios with S^I = .03

the question of selecting the "best" choice is unsettled, one can use the weighting factors for the four basic fitting procedures as a starting point to possibly draw some meaningful conclusions.

The weighting factors for the four fitting procedures discussed in the previous one group study[22] are shown in the following tabulation.

PRO1	least square, no constraint fit	$\gamma = 0.0$
PRO2	ellipsoidal fit	$\gamma = \lambda/\beta^2$
PRO3	combined fit	$\gamma = 1.0$ in (3)
PRO4	fixed square fit	$\gamma = 1/\lambda$

where λ is the La Grange multiplier, and β is defined on p. 65.

The choice of the weighting factor obviously influences how much emphasis one places on the integral or the differential data.

The first question one may raise is what the sign of the weighting factor would be. The answer is definitely positive. The reason is that if one allows a negative weighting factor, one can hypothetically use a large negative number to reduce the function to be minimized in (3) to the minimum value. The solution is of course meaningless since in that case no emphasis is placed on the integral data. Thus only with a discrete choice of a positive weighting factor can one properly weigh the integral term against the differential term to study the error identification.

Furthermore, from the mathematical standpoint, one sees that the four weighting factors for the other basic schemes are nonnegative since the La Grange multipliers of the ellipsoidal fit and the fixed square fit are nonnegative.

The second question one may raise is what is the magnitude of the

weighting factor. Theoretically it can vary from 0 to ∞, deviating from the value of 1 which is the combined fit with an equal weight to the integral and the nuclear data. Since the integral and the nuclear measurements are already weighted by $1/S^I$ and $1/S^\sigma$, respectively in the data fitting, the exact choice of the weighting factor is not apparent, judging from the formalism of the function to be minimized. The choice of 1.0 and 1/G, where G is the number of groups, has been suggested.[11] By varying energy groups from 2 to 4, numerous cases were performed to determine which of these choices seems most appropriate for error identification within the investigated group structure.

The behavior of the weighting factor can be examined as a function of ellipsoidal size. The weighting factor decreases as the size of the ellipsoid, β, increases, due to the fact that the La Grange multiplier does not vary as steeply as the β^2 term and the rate of decreasing of the weighting factor is dominated by the denominator term, β^2. For most cases performed in this study, the La Grange multiplier for the ellipsoidal fit is much less than the term, β^2, and as a result the weighting factor is much less than 1. Since the empirical value of beta equal to 2.5 is usually an appropriate choice, as a beta value in this vicinity often provides the lowest figure of merit, one may feel justified in using this empirical choice of beta. While the outcome of the La Grange multiplier λ for the empirical beta may vary from case to case, the associated weighting factor, obtained from the results in this study, is frequently closer to 1/G than 1. Consequently, within the investigated group structure, the theoretical prediction of 1/G for the weighting factor tends to be con-

sistent with the results in this study, and often gives better results than the choice of 1 for the weighting.

In conclusion, if one utilizes the combined fit for the error identification, the weighting factor of 1/G appears to be the best choice. It seems reasonable that this choice yields better results than the choice of 1, since increasing the number of energy groups, G, automatically puts more and more weight on the cross section data for a weighting factor of 1.0. Unless the 1/G factor is used, the data fitting will be too strongly biased toward the cross section data as the number of unknowns increases with that of energy groups.

Figure 7 shows the general behavior of a weighting factor versus beta.

Topics of Interest

For a better understanding of any result from a fitting procedure, the previous three sections in this chapter are used to define and explain several vital parameters, namely, the figure of merit, the empirical choice of the beta values, the two measures of information, $\overline{\Delta I}$ and $\overline{\Delta I^2}$, and the proper weighting factor, which are in essence the tools for interpreting results of error identification.

Using these tools, one can explore many relevant subjects in error identification, such as the energy dependence, the influence of systematic error, the influence of the uncertainty of assumed errors of nuclear cross sections, the influence of the uncertainty of the assumed statistical errors of integral experiments, the comparison between different types of integral data, and the effect of cross section correlation ratios.

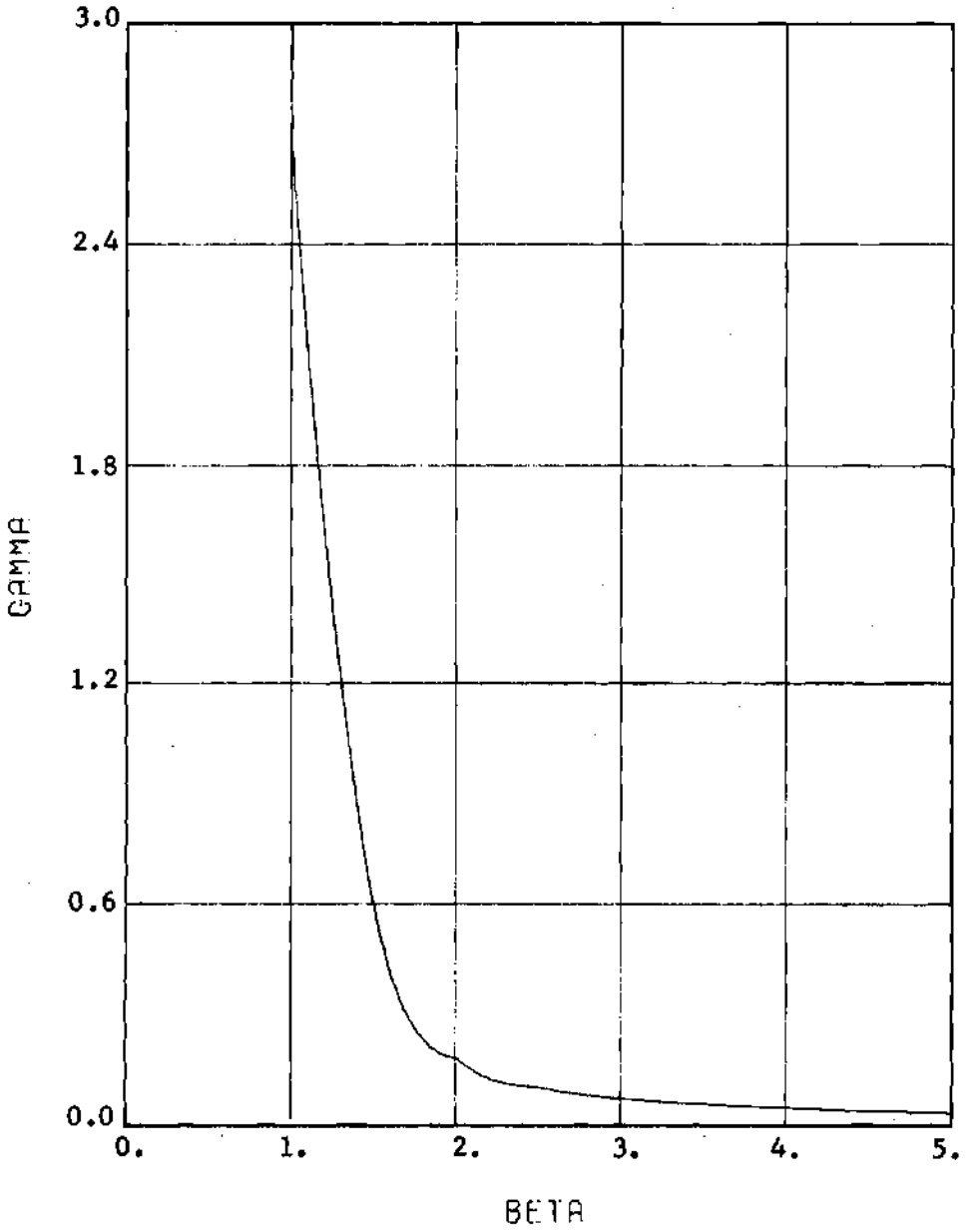


Figure 7. Weighting Factor versus Beta BLACK.2D8T5-2G-FE with 2 Groups, 14 Unknowns, 18 Reaction Rate Ratios with S^I = .03

What follows is the discussion of these topics on error identification, of interest to reactor physicists.

Energy Dependence

One of the principal differences between this study and the previous study[22] of a similar nature is the consideration of the energy dependence up to 4 groups. Even though the reaction rate ratios have been included in addition to the k values as integral data, as the number of groups increases, the number of nuclear unknowns also increases. Although error identification improves as the number of integral data exceeds that of nuclear unknowns, one would like to investigate the multigroup data fitting in the real situation where there is only a limited number of physical assemblies, and the number of nuclear unknowns is often larger than that of integral data. Therefore, many 3 group and 4 group cases in this study are intentionally kept underdetermined.

Most of the 2 group, and some 3 and 4 group cases in this study are overdetermined, and the error identification is quite significant, as shown in Figures 8 and 9. Some of the ellipsoidal cases with reasonable statistical errors of 0.03 for the capture or fission rate ratio, yield figures of merit in the neighborhood of 0.55, that is roughly half of the total error is identified. For the cases with 3 groups, the figures of merit for the optimum beta cases are comparable, e.g. about 0.60 - 0.65. For different numbers of groups, the randomly introduced cross section errors are different, so this small difference in the figure of merit is not significant. For the 3 group case, the number of cross section unknowns identified, that is the unknowns whose individual figures of merit are not 1, is generally also somewhat less than for the 2 group case. The results

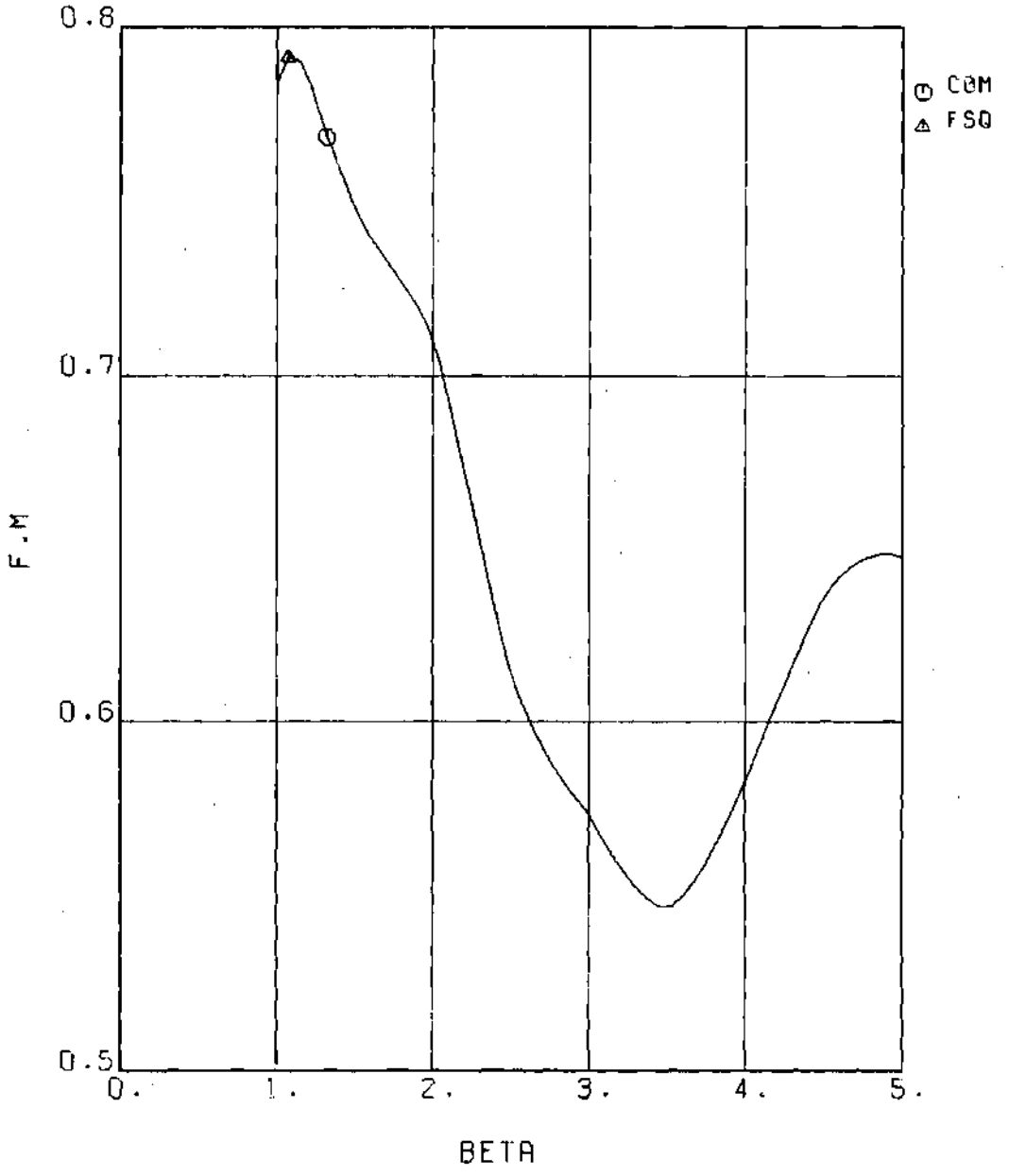


Figure 8. Figure of Merit versus Beta BLACK.2D8T5-2G-FE with 2 Groups, 14 Unknowns, 18 Reaction Rate Ratios with S^I = .03

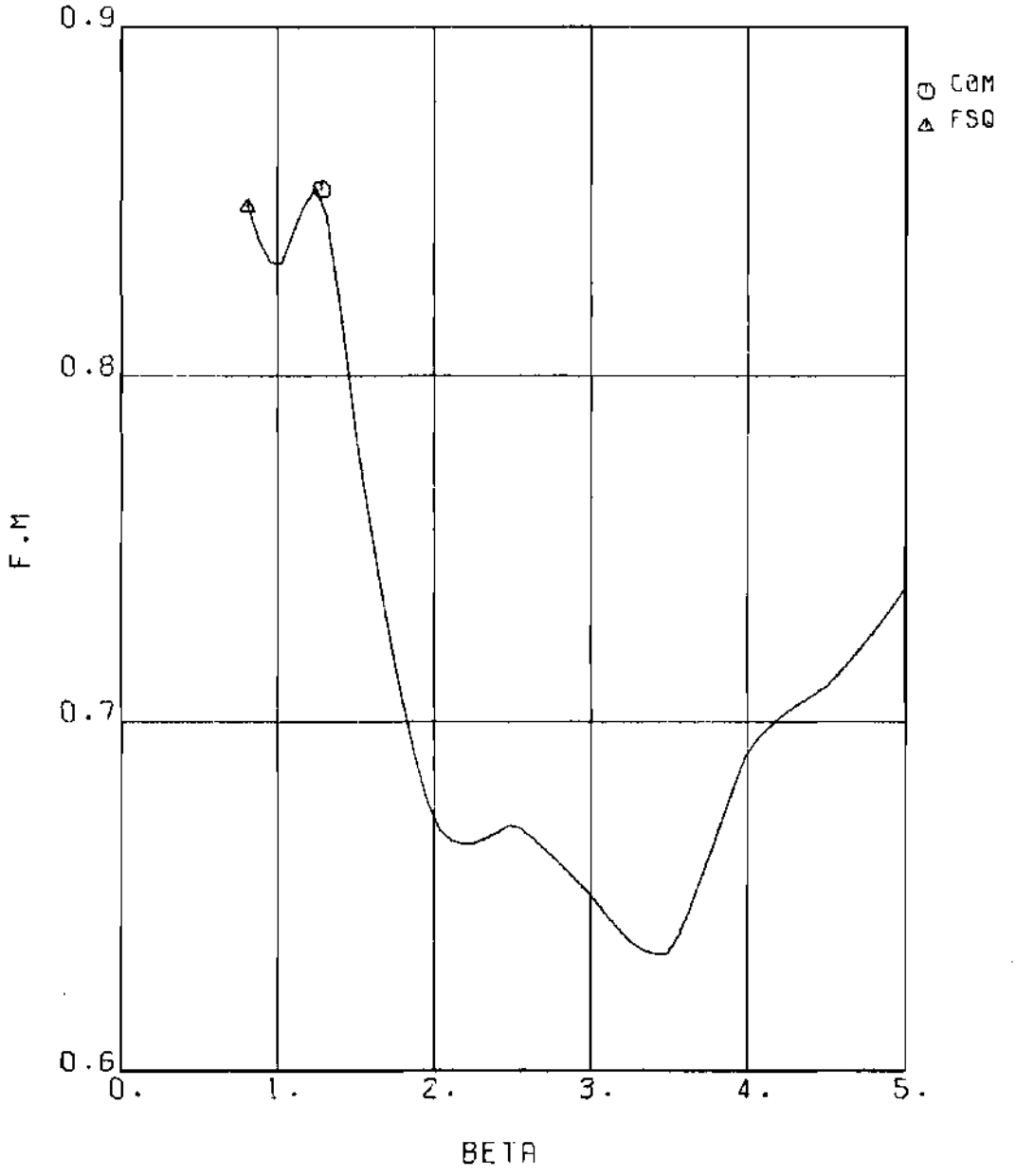


Figure 9. Figure of Merit versus Beta BLACK.3D8T5-3G-FE with 3 Groups, 22 Unknowns, 9 k Values with S^I = .005, 18 Reaction Rate Ratios with S^I = .07

for the 2 and the 3 group cases are shown in Figures 8 and 9.

However, for a typical case of an overdetermined system with 4 groups which has 18 unknowns, 10 k values with the standard deviation of the experimental error $S^I = 0.003$, and 10 fission rate ratios of Pu-240 to Pu-239 with the standard deviation of the experimental error $S^I = .05$, the fitting of the ellipsoidal case, using the empirical beta of 2.5, is still powerful enough to show a figure of merit of .67 with 11 unknowns identified. In this case, since for 7 cross section unknowns their individual figures of merit are 1.0 and for 2 cross section unknowns their individual figures of merit are 0.0, the value of 0.67 for the overall figure of merit indicated more than 0.33 of errors of 11 cross section unknowns is identified. It is interesting to observe that, if one calculates the overall figure of merit using just the well identified variables, the figure of merit would be .46 rather than 0.67. This case is shown in Figure 10.

But with a highly underdetermined case of 30 unknowns, 9 k values with the standard deviation of the experimental error $S^I = .003$, and 9 Pu-240 capture to Pu-239 fission rate ratios with the standard deviation of the experimental error $S^I = .05$, the figure of merit deteriorates to 0.77 with 19 unknowns identified. In this fit, the individual figures of merit for 11 unknowns are 1.0 and for 3 unknowns are 0.0. The overall figure of merit of 0.77 is still an indication of appreciable error identification. If one just uses the well identified variables to calculate the overall figure of merit, it would be .64 instead. This case can be seen in Figure 11.

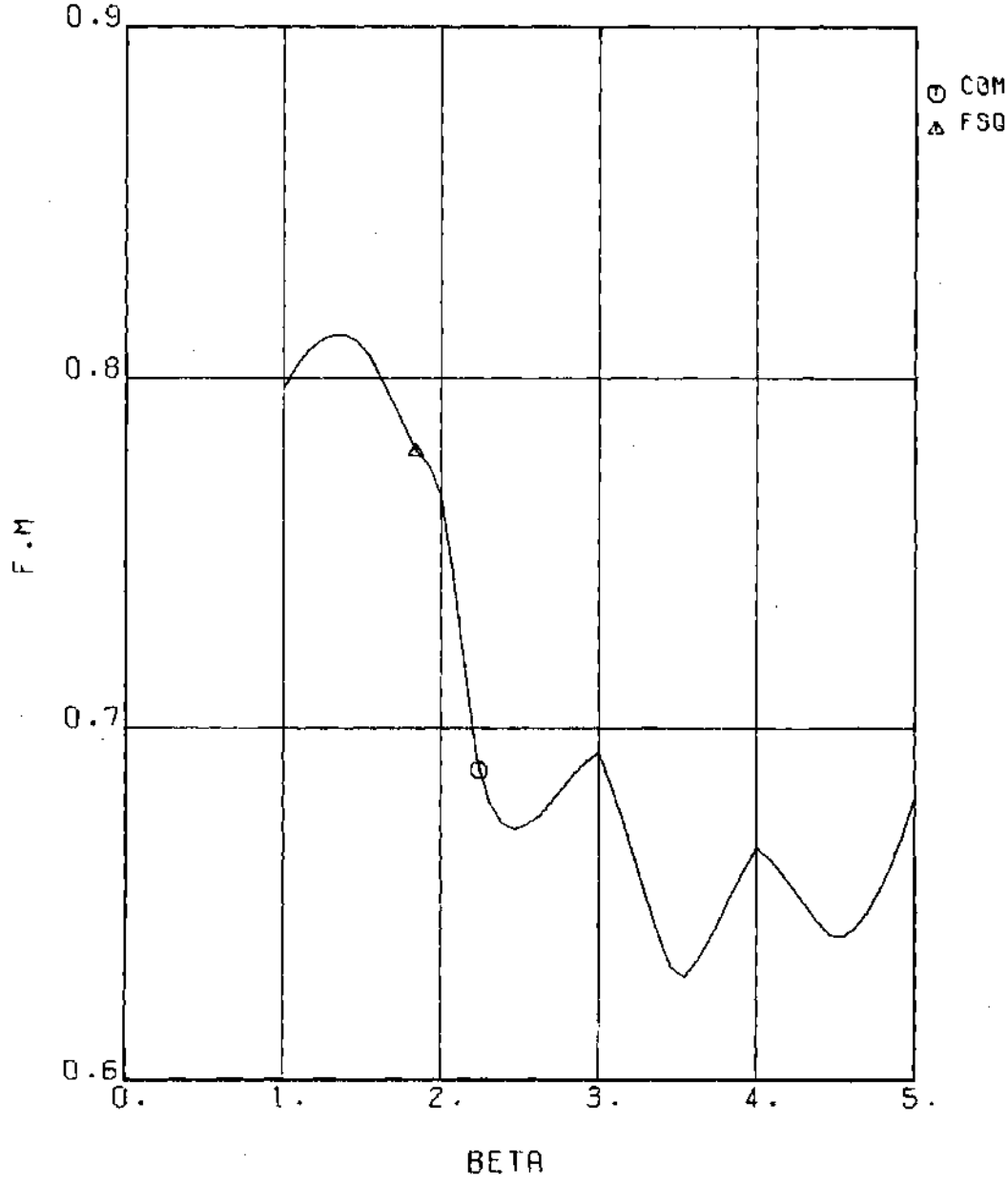


Figure 10. Figure of Merit versus Beta BLACK.DK09FF-4G with 4 Groups, 18 Unknowns, 10 k Values with S_I^I = .003, 10 Reaction Rate Ratios with S^I = .05

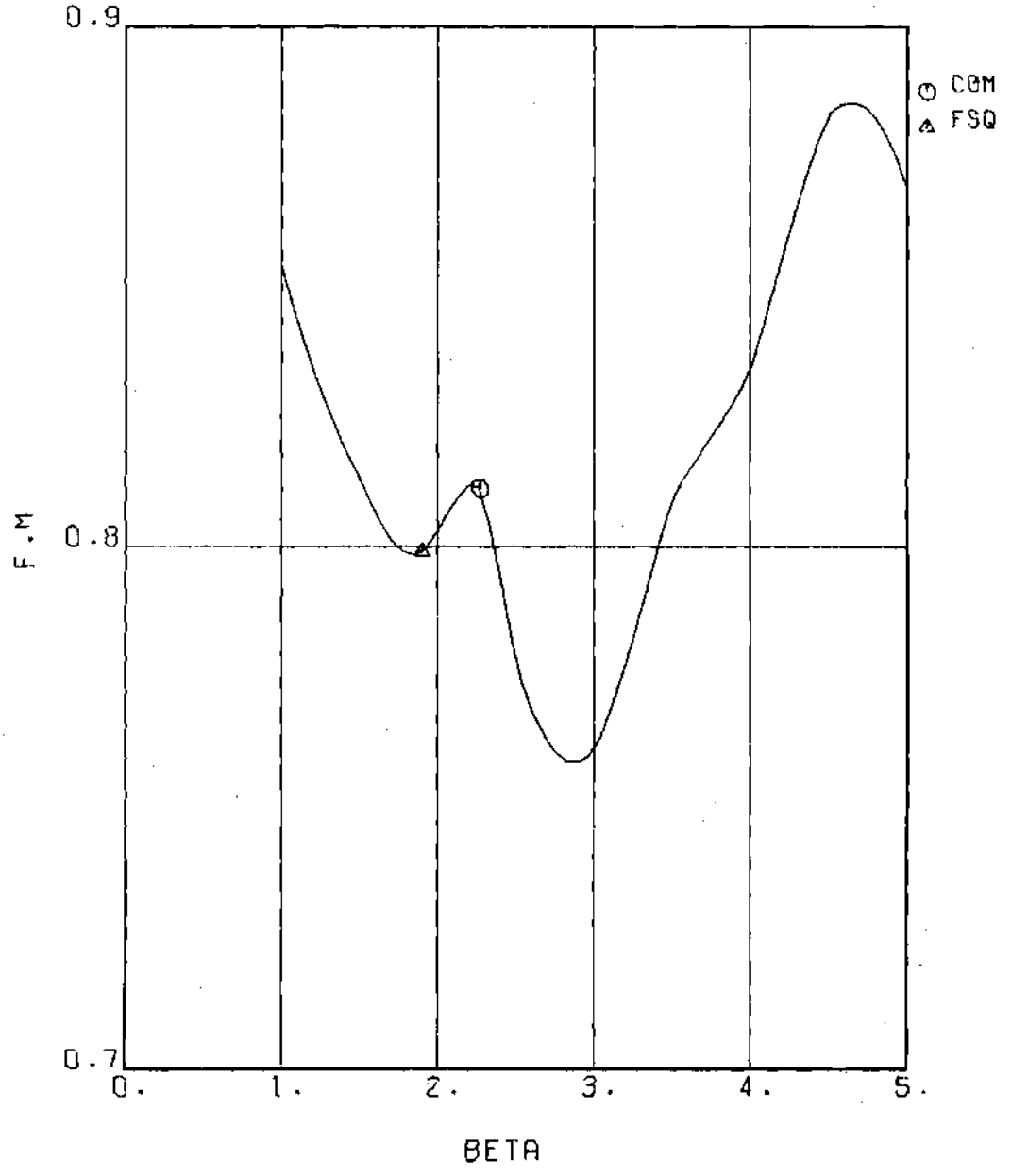


Figure 11. Figure of Merit versus Beta BLACK.DK09CF-4G-FE with 4 Groups, 18 Unknowns, 10 k Values with S^I = .005, 20 Reaction Rate Ratios with S^I = .07

Although one intuitively believes that error identification improves as the degree of overdeterminedness increases, one finds from the cases considered in this study that the results of a barely overdetermined system for the standard least square, no constraint fit are not much different from those of a significantly overdetermined system for the same fit.

To study how the degree of overdeterminedness affects the standard least square, no constraint fit, one can compare the results from three (admittedly highly) overdetermined systems. Appendix G contains the results from these 2 group, 10 unknowns cases. In the fit, .003 is used for the standard deviation of the experimental error of the k values, and .05 is used for that of the reaction rate ratios. Using 10 k values and 20 reaction rate ratios, the figure of merit is .95 with 2 unknowns identified. Utilizing 20 k value and 40 reaction rate ratios, the figure of merit is .89 with 3 unknowns identified, which is still poor error identification. Finally, with 40 k values and 80 reaction rate ratios, the figure of merit decreases to .71 with 6 unknowns identified. It should be pointed out that for these cases with a constraint condition, the error identification would have generally been much better. At any rate, this trend shows that as the degree of overdeterminedness increases, the error identification becomes more significant as shown by the decreasing magnitude of the figure of merit and the increasing number of the errors identified.

Thus the problem of an energy dependent cross section fitting reduces to obtaining more integral data, with sufficient accuracy for the study. As expected, this appears to be the only way to obtain more meaningful solutions. Obviously there will be an upper limit to the number of groups for which the fitting schemes can still produce valuable

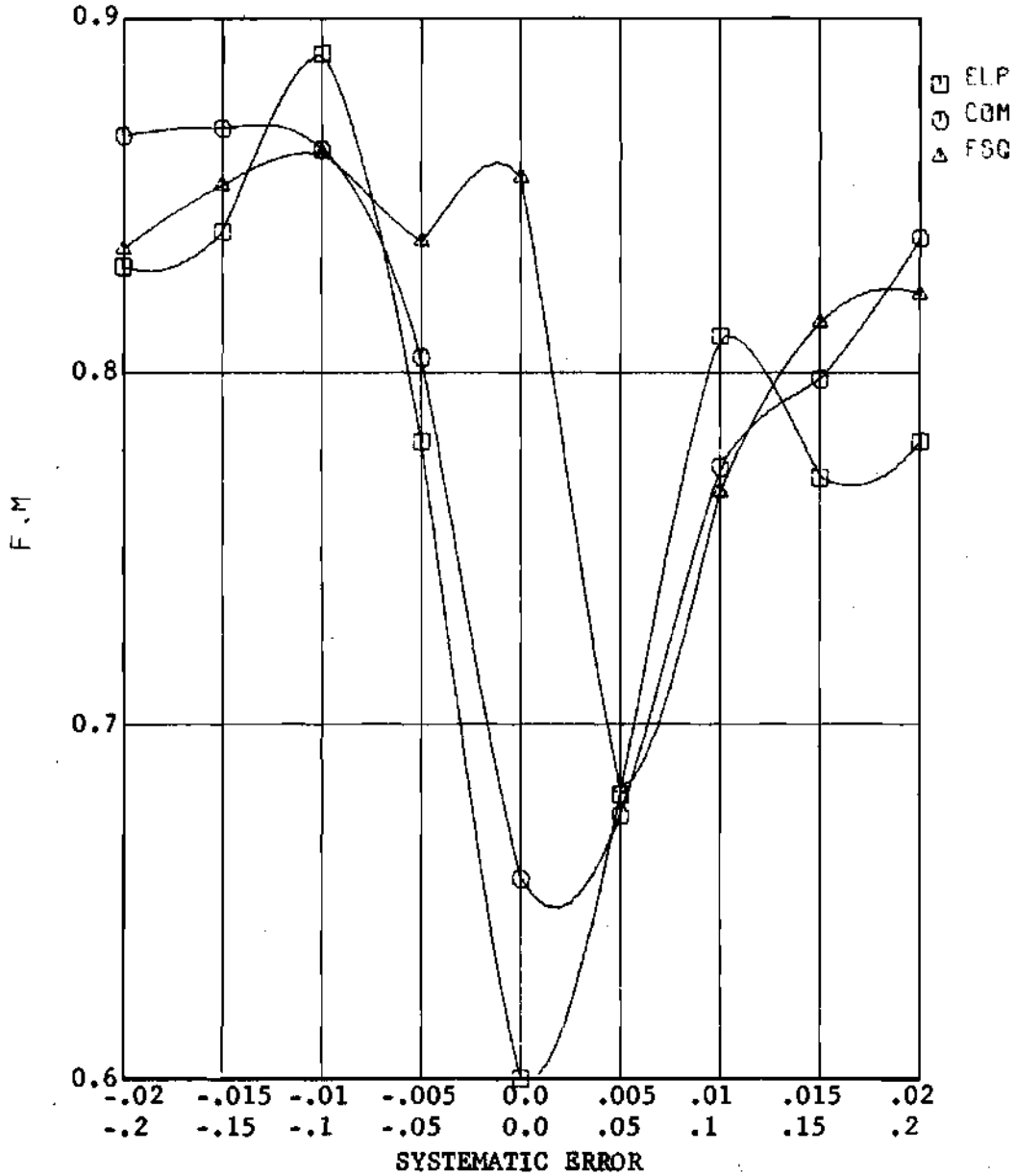
realistic information. From the encouraging results of the cases for up to 4 groups considered in this study, utilizing the k values and the reaction rate ratios, one can still obtain significant error identification for many multigroup cross sections. While in the realistic case one would have more unknowns with four groups, some of the unknowns could be included in a macroscopic effect, to make the case comparable to those considered here. Thus the introduction of energy dependence per se does not inherently prevent cross section error identification.

Influence of Systematic Error

It is possible that there exist systematic errors in any integral experiment, and generally it is difficult to ascertain the exact sign and magnitude of these errors. In the previous cases of data fitting in this work, the systematic errors were not incorporated in the fitting, since no knowledge of their signs and magnitudes is assumed. However, the assumed k and reaction rate ratio errors, which were applied with a statistical variation, ranged up to the values often quoted for the k and the reaction rate ratio errors, including possible systematic errors. In this study systematic errors are also introduced to the fitting schemes, to study their influence on data fitting.

A study was made of introducing systematic errors over a fairly wide range, that is: ±.02, ±.015, ±.01, ±.005 to the k values and ±.2, ±.15, ±.1, and ±.05 to the reaction rate ratios, respectively, for many 3 group cases.

A curve of the figure of merit versus the systematic error for the four fitting procedures is shown in Figure 12 for a typical case. From the curve one observes that for a plausible systematic error approaching



(The top line is for k values, the bottom line is for reaction rate ratios.)

Figure 12. Influence of Systematic Errors BLACK.3D8T5-3G-FE with 3 Groups, 22 Unknowns, 9 k Values with S^I = .001, 18 Reaction Rate Ratios with S^I = .03 (ELP denotes the ellipsoidal fit)

.005 for the k values and .05 for the reaction rate ratios, the figures of merit for the ellipsoidal fit and the combined fit still indicate fairly good error identification; this is in agreement with similar results observed in the one group case.[22] As the systematic errors increase, one expects the error identification to deteriorate. However, at a most unlikely value of +.02 for the systematic error of the k values and a particularly unlikely value of +.2 for the reaction rate ratio, the figure of merit for the ellipsoidal fit is still around .78, which is significantly poorer than for the original value of 0.6. Similar results hold for the 4 group case.

In general one notices that for the cases under discussion the error identification deteriorates more for an introduction of a negative systematic error than that for a positive systematic error. Moreover, for a small positive systematic error of .005 for the k values and .05 for the reaction rate ratios, the error identification is even better for some cases than those without any systematic error. These two phenomena were also observed in the one group study,[22] with no comment. However, upon the close examination of the results in this study, one realizes that the $\overline{\Delta I}$ for these cases without any systematic error is negative. Therefore one suspects that the incorporation of a small positive systematic error might somewhat cancel part of the negative $\overline{\Delta I}$. Since the sign of the $\overline{\Delta I}$, the residue error of the integral data, is determined mainly by a certain combination of the cross sections selected, it is interesting to note that a systematic error with the same sign as the $\overline{\Delta I}$ might do more damage to the error identification than a systematic error with the opposite sign of the $\overline{\Delta I}$.

From the results in this study, it appears that if the systematic errors are of moderate size (e.g. their magnitudes are somewhat less than 0.005 for the k values and 0.05 for the reaction rate ratios), one may obtain good error identification. With systematic errors outside this range, the figures of merit for different fitting schemes tend to deteriorate considerably.

Comparable deterioration was also noted for the previous one group study[22]; however, because of differences in the data for this study and the previous one[22] (less unknowns, larger introduced errors for the important cross sections, etc.), the initial figure of merit for this study is generally much higher than for the previous study.[22] Thus in the previous study,[22] even after introduction of large systematic errors, the error identification was quite good.

Although the figure of merit changes considerably as the magnitudes of the introduced systematic errors increase, the error identification for those variables whose individual figures of merit are not equal to 1 is fairly good. For instance, for the 3 group ellipsoidal case where the systematic error is -0.02 for the k values and -0.2 for the reaction rate ratios, the figure of merit using just the 10 well identified variables is .63 as compared with the overall figure of merit of .83.

Influence of the Uncertainty of Assumed Errors of Nuclear Cross Sections

To investigate how the results from the fitting schemes are influenced by the assumed cross section uncertainties, one assumes a scale factor α^{σ}, multiplies it by S^{σ}, and substitutes S^{σ} by the new product in the fitting procedure while the introduced errors obtained originally from

S^{σ} are kept unaltered. Furthermore, in the calculation of a figure of merit, the S^{σ} is used instead of the product $S^{\sigma}\alpha^{\sigma}$ so that the figure of merit for the fitting schemes will not be influenced directly by a change in the limit given for $0.1S^{\sigma}$ (see p. 63).

Many sets of cases in which α^{σ} is either larger or smaller than 1 were run to study the influence of the uncertainty of the cross section errors. The values in which α^{σ} varies are 0.25, 0.5, 0.75, 1.0, 2.0, 3.0, and 4.0. For the ellipsoidal fit, the empirical choice of 2.5 is used for the beta value.

In general one sees from (2) that the incorporation of α^{σ} into the ellipsoidal fit transforms the ellipsoidal constraint to $(\alpha^{\sigma})^2$ instead of 1.0; therefore, increasing α^{σ} is the same as increasing beta with S^{σ} holding invariant. Consequently, one can expect a usual upside down bell shape curve for the figure of merit versus α^{σ}.

For the fixed square fit, the incorporation of α^{σ} into (4) will reduce the function to be minimized by a factor of $(1/\alpha^{\sigma})^2$ while the fixed square constraint remains intact. As a result the problem is the same as the one without the incorporation of α^{σ}. This can be confirmed by noticing that $\overline{\Delta I}$ and $\overline{\Delta I^2}$ for different α^{σ} in the fixed square fit never change.

Compared with the fixed square fit, the combined fit is naturally more sensitive to the uncertainty of cross section errors since, instead of keeping a value of unity, the weighting factor for the combined fit varies as $(1/\alpha^{\sigma})^2$; nevertheless, compared with the ellipsoidal fit, the magnitude within which the figure of merit varies for the combined fit is much less than that for the ellipsoidal fit primarily because the beta for the combined fit does not change as fast as that for the ellipsoidal fit.

Considering the fact that there is always some uncertainty of the cross section estimated accuracy (S^{σ}) present in any realistic situation, one would prefer using the fixed square fit, at least when considering the influence of this uncertainty, since its results are not influenced by the uncertainty of the cross section accuracy at all. Nevertheless, the generally poor results of the fixed square fit make it less attractive. Furthermore, as one will see in the next section, the fixed square fit is sensitive to another input parameter which contains uncertainty.

As α^{σ} varies from about 0.5 to 2, which is the most reasonable range, for some cases the ellipsoidal fit may yield better results than the combined fit; this depends on where the optimum beta lies. However, as α^{σ} moves outside this range, the combined fit always yields better error identification than the ellipsoidal fit, since the combined fit still considers both the weighting of the S^{σ} and S^{I} terms, but the ellipsoidal fit only considers the effect of S^{σ}.

Varying the energy groups from 2 to 4, one observes a similar trend.

Figure 13 is a typical case which depicts the influence of the uncertainties of cross section errors on fitting procedures.

Influence of the Uncertainty of the Assumed Statistical Errors of Integral Experiments

The statistical errors of the integral experiments are assumed to be known before fitting. To investigate the influence of the values assumed for such errors, one must first multiply the integral errors S^{I} by a common scale factor α^{I}, and then introduce the product as the integral error. However, the integral errors used in the calculation of the dis-

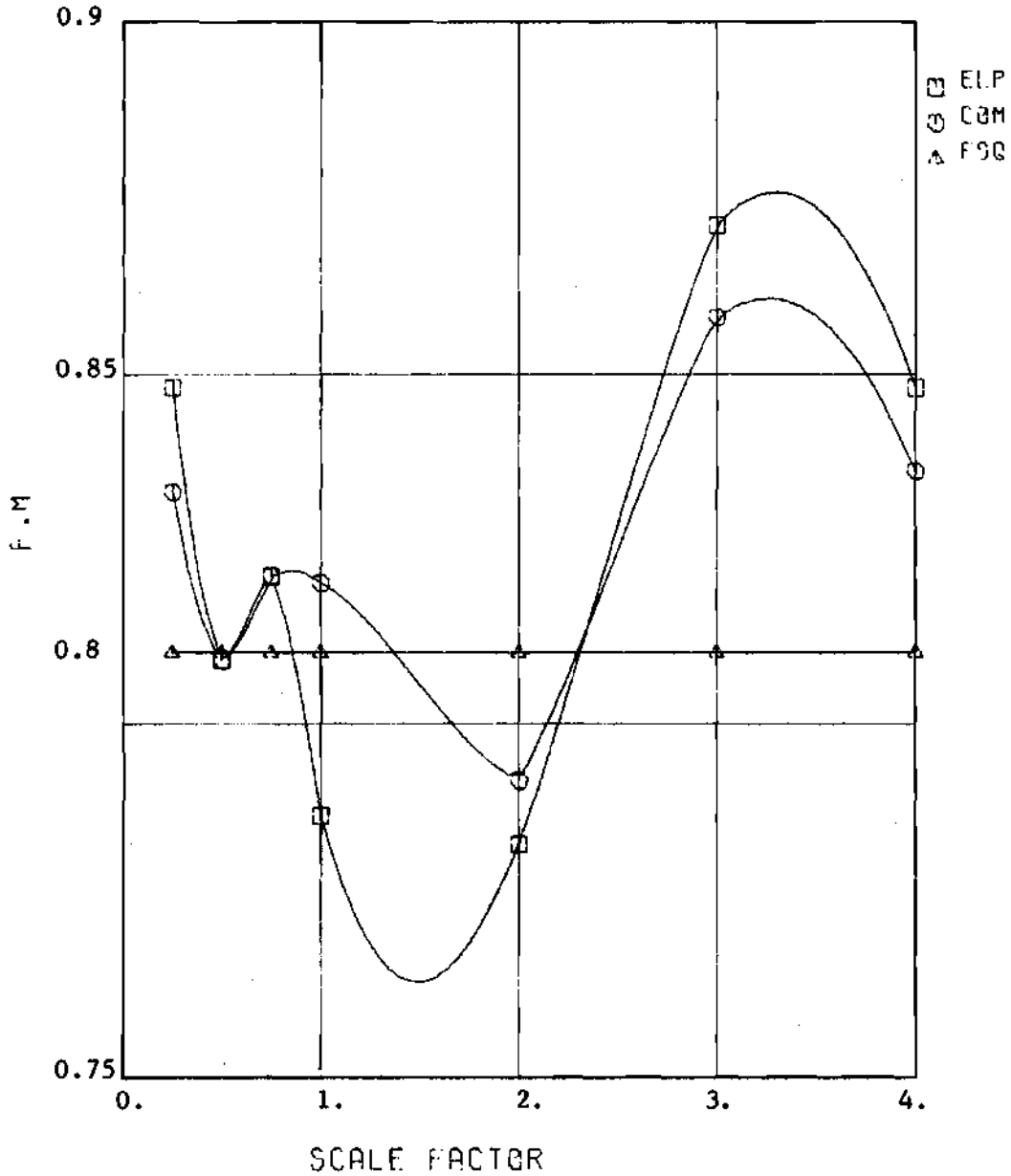


Figure 13. Study of Uncertainty of Cross Sections BLACK.DK09CF-4G-FE with 4 Groups, 30 Unknowns, 9 k Values with S^I = .003, 9 Reaction Rate Ratios with S^I = .05

crepancies between the theoretical and the experimental integral data remain unchanged.

Many sets of cases were performed in which the scale factor was varied from 0.25 to 4.0. For the ellipsoidal fit, the empirical choice of 2.5 was used for the beta value.

The results verify that the ellipsoidal fit for different values of α^I yields the same figure of merit; this is expected, since the ellipsoidal fit is independent of the uncertainty of the assumed statistical errors, as one can see from (2). The reason is that the contribution of α^I to the ellipsoidal fit only reduces the function to be minimized by a factor of $(1/\alpha^I)^2$ and the fit is not influenced at all; thus the minimizing problem is not altered.

The fixed square fit is the procedure which should be most sensitive to the assumed uncertainties of the integral data errors. With the introduction of α^I to (4), the constraint is changed from 1.0 to $(\alpha^I)^2$. Thus the outcome of the fitting would vary according to the size of the constraint. It is instructive to observe that for much less than 1, the constraint of the fixed square fit is so small that the identified errors are too large to offer any meaningful identification. This is equivalent to the "overfitting" of the integral data in the standard least square, no constraint fit. The behavior of overfitting in the fixed square fit for small α^I has also been observed in the previous one group study.[22]

As α^I increases, the weighting factor for the combined fit increases as $(\alpha^I)^2$; therefore, compared with the ellipsoidal fit, the combined fit is more sensitive to the uncertainty of the statistical errors of the integral data.

If one compares the combined fit with the fixed square fit, one observes that at $\alpha^I = 1$, a realistically possible change of 50% in α^I would increase the figure of merit for the fixed square fit to 1, which is the indication of the worst error identification. However, the figure of merit for the combined fit in this range of α^I does not vary as drastically as that for the fixed square fit. This is due to the reason that as α^I decreases below 1 the combined fit still considers the weighting effects of both the S^I and S^σ terms whereas the fixed square fit is in essence considering the weight of S^I only.

From all the cases considered in this study, one consistently observes the similar behavior of the poor error identification of the fixed square fit in the region where α^I is somewhat less than 1.

Due to the presence of the uncertainty of the assumed statistical errors of the integral data and that of the cross sections, one may often choose the combined fit primarily because it is not as sensitive to the uncertainty of the assumed statistical errors of the integral data as the fixed square fit, and not as sensitive to the uncertainty of the cross section estimated accuracy as the ellipsoidal fit.

Figure 14 is a typical example of what has been discussed.

Comparison between Different Types of Integral Data

The error identification in cross sections is obviously dependent on the type of the integral data employed. For instance, if one wishes to identify errors only in the cross sections important for breeding, one should use the reaction rate ratios involving the significant cross section values in the fit since the reaction rate ratios are more sensitive to the changes in these cross sections used in the breeding than the k

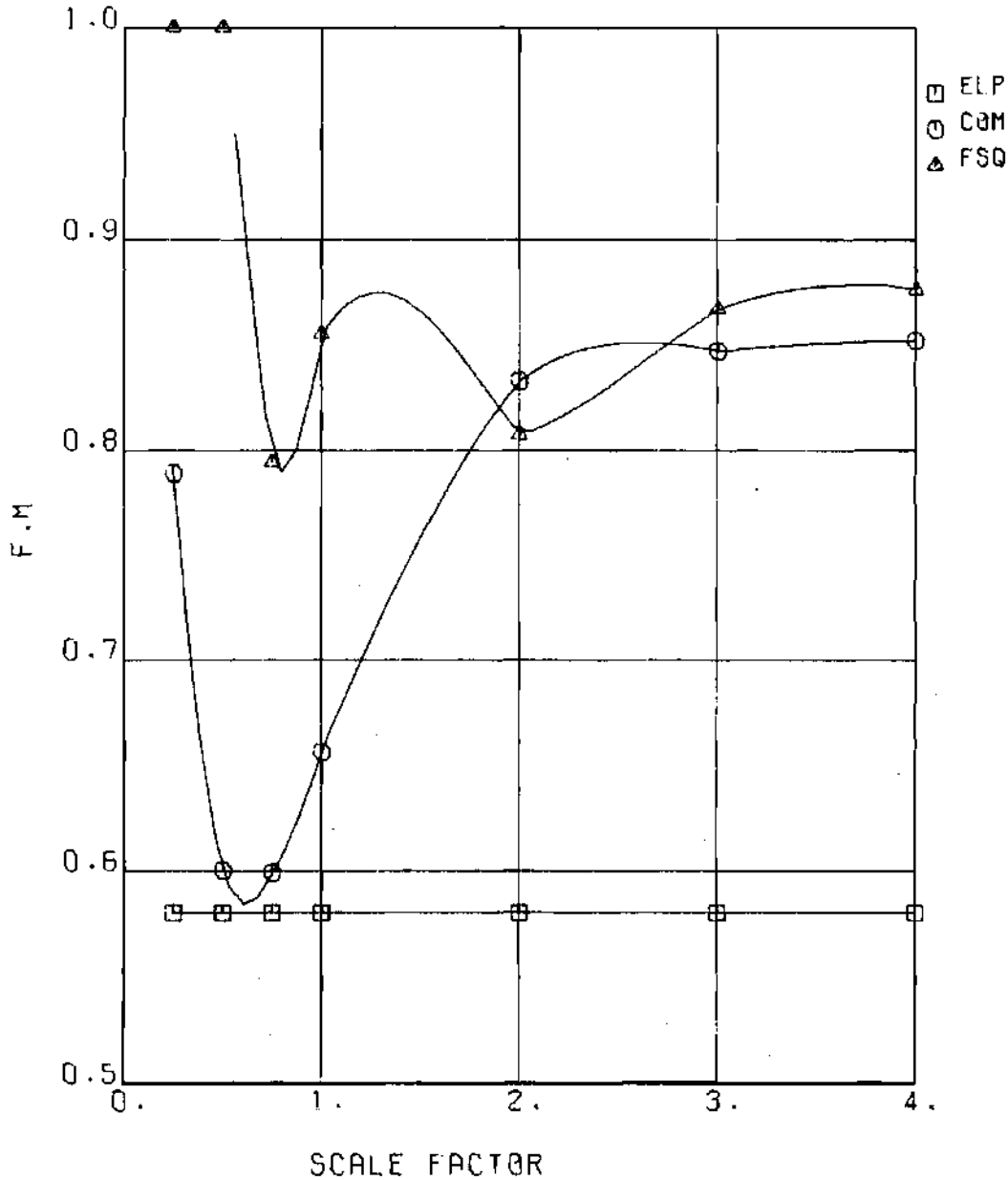


Figure 14. Study of Uncertainty of Integral Data BLACK.3D8T5-3G-FE with 3 Groups, 22 Unknowns, 9 $\underline{k}$ Values with S^I = .001, 18 Reaction Rate Ratios with S^I = .03

values. Similarly, if one wishes to identify errors in the cross sections important for criticality, one should use the k values. Furthermore, one suspects that, if one uses a mixture of the k values and the reaction rate ratios rather than only one type of integral data, one might obtain better overall error identification.

Many cases were run to compare two different combinations of integral data. For example, one is with 9 k values, and 9 values of Pu-240 capture to Pu-239 fission rate ratios while another used 18 reaction rate ratios, which includes 9 values of the Pu-240 fission to Pu-239 fission rate ratio, and 9 values of the Pu-240 capture to Pu-239 fission rate ratio. The influence of the different types of integral data can be seen by comparing Figure 15 with Figure 16.

In many cases with .005 for the standard deviation of the experimental error of the k value and 0.07 for that of the reaction rate ratio, the figure of merit is a few percent less than that for those cases in which only the reaction rate ratios with 0.07 for the standard deviation of the experimental error are used. For example, when one examines the 3 group ellipsoidal fit with the beta value of 2.5, one observes that even the individual figures of merit for the important cross sections for the case which uses the k values and the reaction rate ratios are a few percent less than those for the case which uses the reaction rate ratios only. Appendix G contains the results of these two cases.

For other values of S^I, the standard deviations of the statistical errors of the experimental integral data, and a large number of cross sections in the fitting, one still observes that the combination of k values and reaction rate ratios yields a better overall figure of merit than for

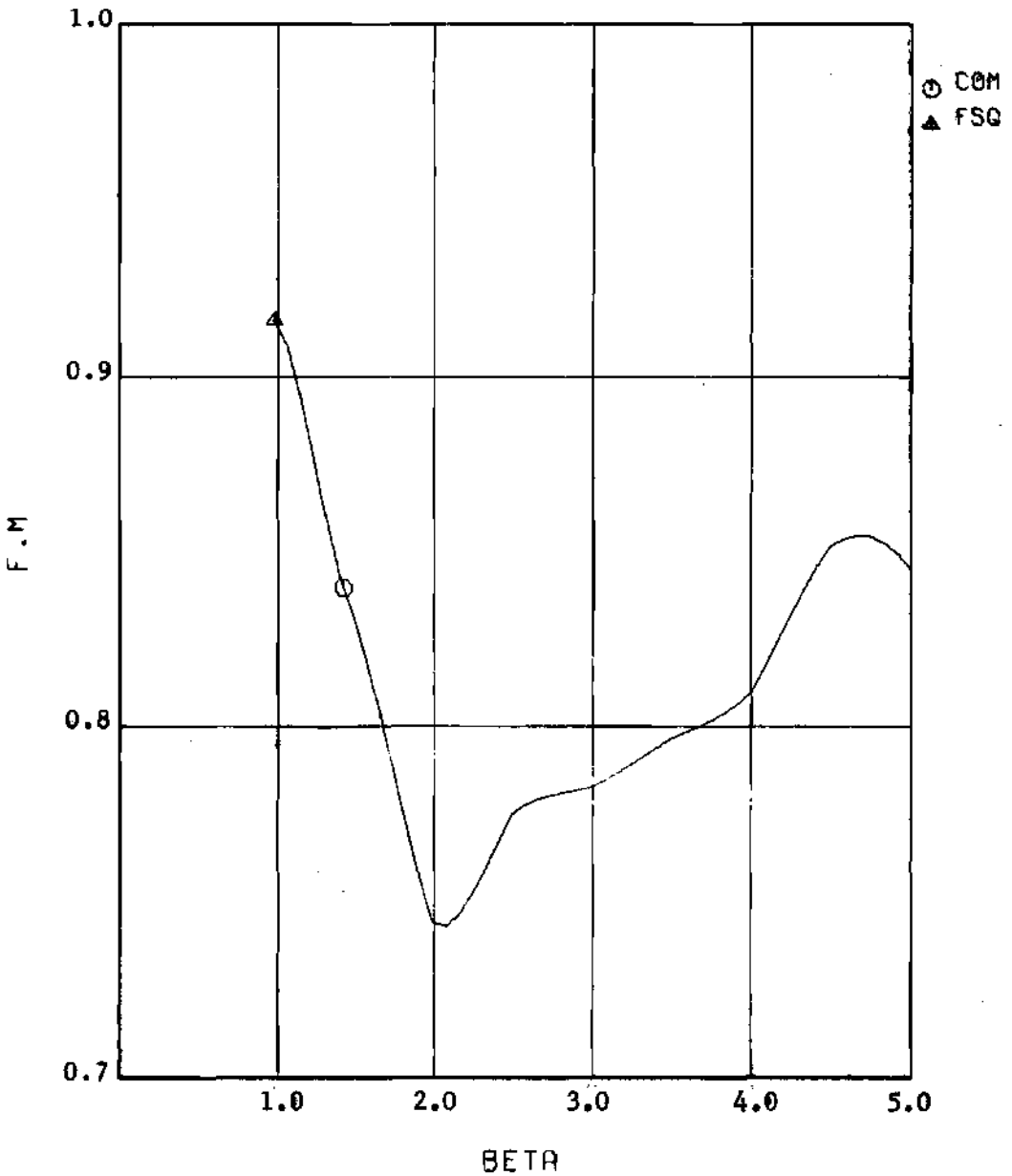


Figure 15. Figure of Merit versus Beta BLACK.DK09CF-3G-FE with 3 Groups, 24 Unknowns, 9 k Values with S^I = .005, 9 Reaction Rate Ratios with S^I = .07

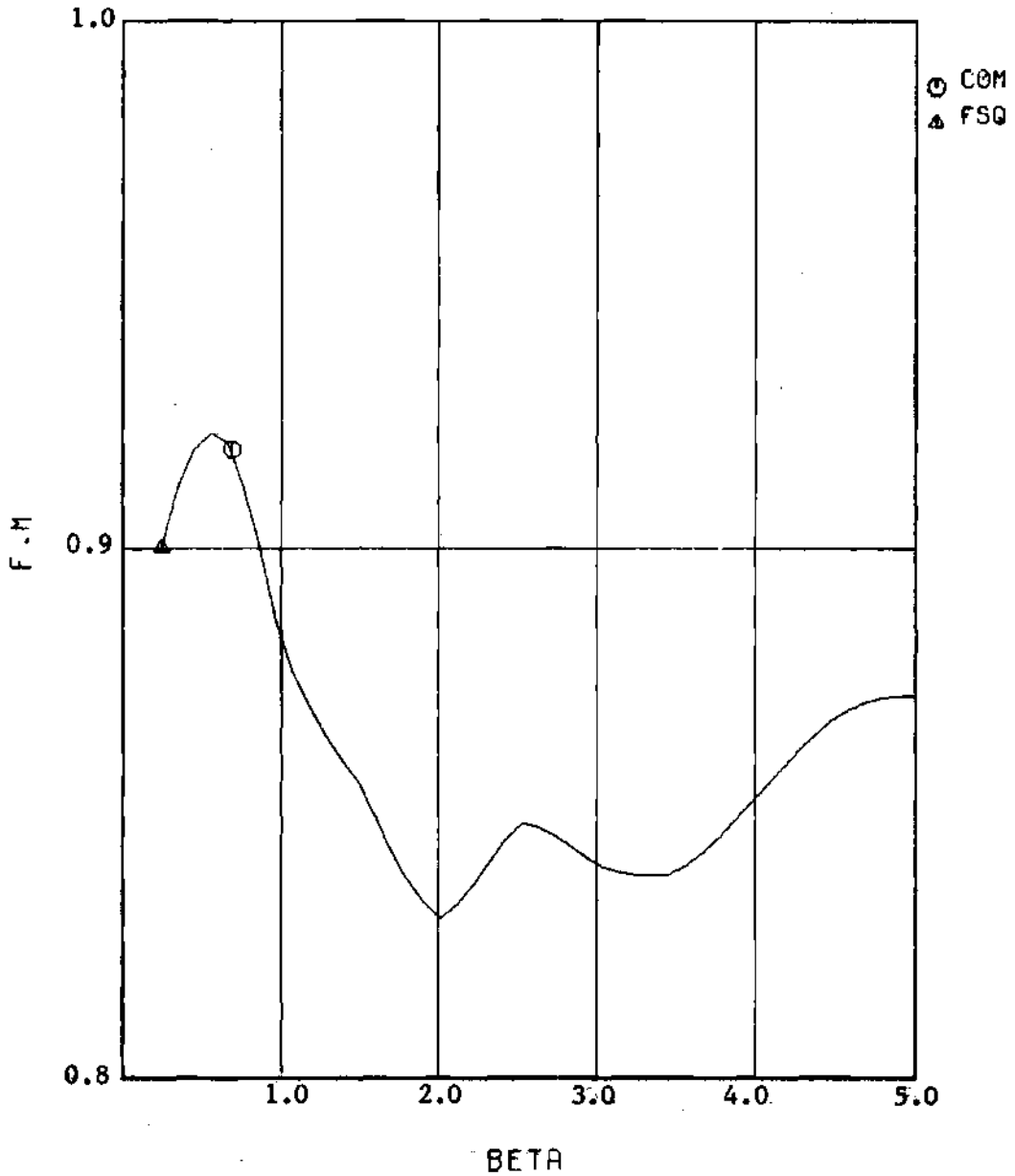


Figure 16. Figure of Merit versus Beta BLACK.2DOT9-3G-FE with 3 Groups, 24 Unknowns, 18 Reaction Rate Ratios with $S^I = .07$

the use of reaction rate ratios only. For instance, a case using both types of integral data with S^I of .003 and .05 for the k and reaction rate ratios, respectively, produced a better overall figure of merit than a case using the same number of integral data, but only k values, with the same S^I. Similarly, a case using k and reaction rate ratios with S^I of .001 and .03, respectively, gave a better figure of merit than when only k values with the same S^I were used. Varying the number of energy groups up to 4, one notices the same behavior as that which has been discussed. From the cases considered in this study, it appears that one should use a mixture of integral data (i.e. the k values and the reaction rate ratios) instead of only one type of integral data, to obtain better error identification.

Study of Cross Section Correlation Ratios

To study the effect of the cross section correlation on the error identification, one has to compare two cases:

(1) Use the correlation to introduce the nuclear errors such as $\Delta\sigma_f$ and $\Delta\alpha$ into the fitting scheme. Then use a data fitting to identify the errors in $\Delta\sigma_f$ and $\Delta\alpha$. Finally calculate the corresponding figure of merit.

(2) Use the correlation to first produce the nuclear errors $\Delta\sigma_f$ and $\Delta\alpha$ whose magnitudes are identical to the errors introduced in case (1). Before the fitting, use these two errors to calculate the related $\Delta\sigma_c$, and then introduce $\Delta\sigma_f$ and $\Delta\sigma_c$ into the fitting scheme. From the identified $\Delta\sigma_f$ and $\Delta\sigma_c$, which are identified without considering correlation, then calculate the related $\Delta\alpha$ and the figure of merit.

The expression for $\Delta\sigma_c$ can be derived as follows:

From the definition of α, one observes

$$\alpha = \frac{\sigma_c}{\sigma_f} \tag{36}$$

Similarly one acknowledges

$$\alpha + \Delta\alpha = \frac{\sigma_c + \Delta\sigma_c}{\sigma_f + \Delta\sigma_f} \tag{37}$$

Using (36) to simplify (37), one obtains an expression which offers all three types of errors in percent

$$\frac{\Delta\sigma_c}{\sigma_c} = \frac{\Delta\alpha}{\alpha} + \frac{\Delta\sigma_f}{\sigma_f} + \left(\frac{\Delta\alpha}{\alpha}\right)\left(\frac{\Delta\sigma_f}{\sigma_f}\right) \tag{38}$$

If one takes the partial derivative of α with respect to σ_c and σ_f for the first order approximation, one obtains the expression which is identical to the first two terms on the right hand side of (38). The expression for the first order approximation can also be derived by first equating (29) to (30), and then cancelling the sensitivity coefficients. Thus (38) which in addition includes a cross product term is more refined than the first order approximation and is used in this study.

Since one pretends in case (2) that one does not know any correlation is present, the comparison of case (1) with case (2) will indicate the effect of neglecting the cross section correlation on the error identification.

Many sets of cases were performed to investigate the effect of the correlation. One can study a typical example shown in Table 12. In general, the figure of merit for the case which pretends no correlation exists falls in the range where the figure of merit for the correlated case exists. Since there is not much difference of magnitude between the figures of merit for these two cases, one can conclude that one can obtain good results in the error identification without considering the cross section correlation ratios, as long as the standard deviation of the experimental integral data are reasonably small. However, as the standard deviation of the experimental integral data increases significantly, the error identification using the correlation ratios tends to yield better results than that without any correlation.

Table 12. Comparison Between the Correlated and Uncorrelated Cases with BLACK.DK09CF-4G-FE

Fitting Scheme	Beta	Correlated F.M	Uncorrelated F.M	S^I
ELP	2.5	.77	.74	.001
COM	1.95	.81	.76	.03
FSQ	1.54	.78	.75	
ELP	2.5	.74	.78	.003
COM	1.86	.73	.73	.05
FSQ	1.23	.75	.75	
ELP	2.5	.74	.84	.005
COM	1.61	.75	.82	.07
FSQ	1.03	.81	.81	

Note: F.M is the Figure of Merit.
S^I is the statistical error of experimental integral data.
The correlated figure of merit is related to case (1) on p. 98.
The uncorrelated figure of merit refers to case (2) on p. 98.

CHAPTER VI

EPILOGUE

Conclusions and Recommendations

The error identification in various fitting procedures can be unified by varying the size of the ellipsoidal constraint. As many evaluations show, there is an optimal ellipsoidal size which, while differing from case to case, generally falls in the vicinity of 2.5.

For any given set of data, there exists also an optimal weighting factor between the integral and the differential influence. The optimal weighting factor always corresponds to the optimal ellipsoidal size. Since in the realistic situation one has no prior knowledge of the optimal beta, the associated weighting factor is not known. However, for the cases considered in this study, the weighting factor of 1/G where G is the number of energy groups, generally gives better error identification than a weighting factor of 1.0.

The results of the four fitting schemes verify the following:

(i) Unless one has a much larger number of integral data than that of cross sections, the figure of merit obtained in the standard least square, no constraint fit is always in the neighborhood of 1, i.e. the error identification is poor.

(ii) For the underdetermined case of the standard least square fit, there exists a unique solution if one redefines the problem and uses

the pseudoinverse in the solution; nevertheless, this solution is generally not helpful in the error identification.

(iii) Many cases of the standard least square, no constraint fit correspond to an "overfitting" of the integral data, for which poor error identification is expected.

(iv) Based on the above results, the use of the standard least square fit is generally not feasible for multigroup data fitting to identify cross section errors.

(v) In general the beta which gives the same result for the fixed square fit is less than that for the combined fit with the weighting factor of 1. That is, the beta for the fixed square fit is on the left hand side of the beta for the combined fit in the figure of merit versus beta curve. A similar trend was also observed in the previous one group work.[22] Furthermore, the figure of merit for the fixed square fit is often higher than that for the combined fit. Therefore, the result from the combined fit is often more meaningful than that from the fixed square fit.

(vi) The beta for either the fixed square fit or the combined fit with the weighting factor of 1 usually lies on the left hand side of the minimum in the figure of merit versus beta curve. Thus the optimal beta gives better error identification than the other fitting schemes.

(vii) The figure of merit versus beta curve is usually an upside down bell shape, even though the figure of merit is defined differently from that in the previous one group work.[22] This is expected since any other result would indicate a poor definition of the figure of merit. A similar shape was observed using the definition of the figure of merit

from the previous work.[22]

From the results obtained in this study, the figures of merit are much higher than those in the previous one group work.[22] The main reason is that, in this study, a more systematic method of introducing errors is incorporated to ensure that the introduced errors are random in nature. As a result, there are more small introduced errors than in the previous one group work.[22] The figures of merit tend to increase as the number of small introduced errors increases, primarily because the fitting procedures will have more difficulty in identifying small introduced errors than the large ones.

In general it is difficult to define a figure of merit which will give the proper credit to the small introduced and identified errors. In this study a value of 0.1 S^{σ} was used for the definition of a small introduced error, and to indicate good error identification the identified error was required to be within this value of the introduced error.

With the figure of merit used in this study, a value greater than 0.85 generally indicates poor error identification. However, even in this range the error identification for some important cross sections may still be significant. Further, if one is willing to relax the above mentioned limit of 0.1 S^{σ} for identification of small errors, the figure of merit improves. Many of the introduced and identified errors, while not meeting this limit, are still relatively small and might be considered as good error identification.

(viii) The ellipsoidal fit with the empirical choice of 2.5 for the optimal beta frequently yields better results than the fixed square fit or the combined fit with the weighting factor of 1.

(ix) In case the statistical errors of the integral data are estimated much too low, the result from the fixed square fit is identical to that from the overfitting in the standard least square, no constraint fit.

(x) Since the combined fit is not as sensitive to the influence of the uncertainty of the assumed errors of the cross sections as the ellipsoidal fit, and not as sensitive to the influence of the uncertainty of the statistical errors of the integral data as the fixed square fit, the combined fit should be used in a fitting if the uncertainty of either the assumed errors of the cross section or the statistical errors of the integral data is not known reasonably well.

(xi) Generally speaking, if the systematic errors are moderate in size, their influence on the error identification is not large. Thus if the particular combination of integral data being used gives good error identification without systematic errors, this will still be the case when moderate systematic errors are introduced. For systematic errors greater than about .005 and .07 for k and reaction rate ratios, respectively, the error identification can deteriorate considerably.

(xii) The two measures of information $\overline{\Delta\rho}$ and $\overline{\Delta\rho^2}$ defined in the previous one group work[22] for one type of integral data can be redefined as $\overline{\Delta I}$ and $\overline{\Delta I^2}$ and applied to a combination of various integral data. Since the purpose of these two measures of information is to indicate how many residue errors of the integral data are left after the data fitting, the two measures in general will decrease in absolute magnitudes as beta increases. As beta reaches that for the standard least square, no constraint fit, $\overline{\Delta I^2}$ reduces to a minimum which signifies that the fitting

may be overdone.

(xiii) Though the error identification is generally improved by an increased accuracy of the experimental integral data, its effect is not as remarkable as shown in the previous one group study.[22] This is believed to be mainly due to the fact that the number of unknowns used in this study is larger than that in the previous one group work.[22] Some cases with extremely small standard deviations of the experimental integral data were run to check the programs. The results showed that the error identification is improved tremendously as expected; most of the identified errors have the same signs and magnitudes as the introduced errors.

(xiv) The error identification is often improved by the overdeterminedness of the system, though this effect is not as conspicuous as that in the one group work.[22] Despite the fact that the solution from a barely overdetermined system is not as accurate as the one from a highly overdetermined system, in most cases the barely overdetermined system already gives satisfactory results if a reasonably small accuracy is assumed for the uncertainty of the experimental integral data.

(xv) Judging from the results in this study, if the integral data are known fairly accurately, one does not have to use the cross section correlation ratios to obtain good results in the error identification in a data fitting; the fit without the consideration of the cross section correlation ratios often yields the equivalent result as that with the consideration. Nevertheless, as the statistical error of the integral data is increased, the influence of including the correlation in the fit becomes more significant.

(xvi) For the cases considered in this study, one often obtains better overall error identification if one uses a mixture of the k values and the reaction rate ratios instead of only one type of integral data.

(xvii) Using the k values and the reaction rate ratios, one can obtain good results in the error identification up to 4 groups for many cross sections.

As shown in this study, the inclusion of energy dependence per se does not seem to be a major obstacle; the real problem is how to maintain the number of the integral data comparable to that of the differential data. Therefore, it appears that, for a meaningful error identification, one cannot expand the number of energy groups too largely.

(xviii) If the integral data and the nuclear unknowns one deals with in a fit are considerably different from those in this study, one may use the ellipsoidal fit to perform an appropriate set of gedanken experiments to determine the optimal beta.

The following is a list of pertinent recommendations for further research.

1. Incorporate the space dependence into the fitting schemes and the calculation of sensitivity coefficients.

2. Study the influence of other cross section correlations such as that between adjacent groups.

3. Study more accurate methods of calculating the sensitivity coefficients, such as higher order perturbation theory,[42] and the variational approach.[43]

APPENDIX A

EXISTENCE OF SOLUTION FOR A CONSTRAINED FIT

When attempting to solve a fitting procedure with a constraint, one generally considers the solution of a comparable problem with the aid of a La Grange multiplier.

However, the question must still be raised as to whether the solutions for these two problems are identical. The following treatment is to clarify this doubt and ensure that under the specific nature of this study these two problems are indeed equivalent.

To elaborate this point, one first defines the following two problems: 1) Problem I. Find x which minimizes f(x) subject to $g(x)-a = 0$

2) Problem II. Find the critical points of F where

$$F(x) = f(x) + \lambda(g(x)-a)$$

x is a shorthand notation for $x_1, x_2, \ldots, x_k$

f, g, and F are functions of x

λ is a La Grange multiplier.

Any set of x and λ which satisfies the following two equations simultaneously is called a critical point of F.

$$\nabla_x F = 0$$

$$\nabla_\lambda F = 0$$

where ∇_x is a shorthand notation for taking partial derivatives with respect to x.

The function F, which contains a variable λ and functions f and g as in Problem I, is sometimes called the Hamiltonian function.[24]

If there is a solution of Problem I, it is possible that none of the critical points of Problem II solves Problem I.[24] However, if f and g are both of nonnegative quadratic form which can be expressed as convex functions in some coordinate systems, there will be only one critical point of F.[24] Moreover, knowing that there is a solution of Problem I, one would like to conclude that the critical point of F solves Problem I. This is indeed true as shown in the following lemma.[40]

Lemma: If X_o minimizes $f(x)$ subject to $g(x) = 0$, then there is a λ_o such that (λ_o, X_o) is a critical point of $F(x)$ where $F(x) = f(x) + \lambda g(x)$

Since the functions to be minimized and their related constraints in the fitting procedures satisfy the nonnegative quadratic form, one can solve the critical point of the equivalent Hamiltonian functions for data fitting.

The question which remains to be answered is under what condition can one evaluate the desired critical point with ease. Fortunately the Kuhn Tucker conditions[41] state that, if both f and g are of nonnegative quadratic form, the λ which solves Problem II will be nonnegative. This is extremely helpful in carrying out a trial and error solution primarily because one can concentrate the search for λ in the positive region only.

APPENDIX B

RANDOM SAMPLING FROM A STANDARD GAUSSIAN DISTRIBUTION

Random sampling from a Gaussian distribution is usually a difficult task. However, taking advantage of the Central Limit Theorem,[23] one can sample from a uniform distribution to approximate the Gaussian distribution.

The Central Limit Theorem[23] states that, if $\bar{X}_n$ is the mean of a random sample of a size n from a density f(x) which has mean μ and variance σ^2, and if one defines a new random variable y_n by $y_n = [(\bar{X}_n-\mu)/\sigma]n^{1/2}$ then the distribution of y_n approximates the Gaussian distribution with mean 0 and variance 1 as n increases.

The beauty of this theorem is the freedom that any distribution will accomplish the same purpose. In reality the easiest choice is of course the uniform distribution.

Thus if n independent X_i are randomly sampled from a uniform distribution on [0,1], one can first calculate the expected value and the variance of each selected random number as follows:

$$E X_i = \int_0^1 x \, dx = \frac{1}{2}$$

$$\mathrm{Var}\, X_i = E X_i^2 - (E X_i)^2 = \frac{1}{12}$$

Similarly one can produce the expected value and the variance of the sum of these n random numbers.

$$E\left[\sum_i^n x_i\right] = \frac{n}{2}$$

$$Var\left[\sum_i^n x_i\right] = \frac{n}{12}$$

Then applying the Central Limit Theorem,[23] one forms the new random variable,

$$y = \frac{\sum_i^n x_i - \frac{n}{2}}{\sqrt{\frac{n}{2}}}$$

whose distribution will approach the standard Gaussian distribution as n increases.

To facilitate the sampling of y, one can use 12 as a possible choice of the sample size to reduce the denominator of the expression of y to 1.[24] Hence one obtains

$$y = \sum_i^{12} x_i - 6 \tag{39}$$

To check whether the sample size of 12 is sufficiently large for a good approximation, one can use the true distribution of the y and calculate the probability of obtaining a sampled value from a fixed interval. Then one can compare the evaluated probability with that from the true Gaussian distribution in the same interval.

Using a fixed interval from 0 to 1, the difference between these two values of probability is less than 0.6 percent. Therefore, one can safely conclude the sample size of 12 is adequate for a reasonable approximation.

Though (39) is a working formula for sampling from a standard Gaussian distribution, the next question is how to sample from a uniform distribution. Fortunately the UNIVAC routine RANDU[38] is available for this purpose. Compared with the true uniform distribution, the routine RANDU is shown[38] to be accurate to $1/2^{27}$.

APPENDIX C

DERIVATION OF THE VARIANCE COVARIANCE FORMULA

Given: $$\hat{u} = UQ^{-1}y \tag{40}$$

Show that $\psi = UQ^{-1}U^T$ where all the variables satisfy (5).

Proof: Since $$Y = Hu + \epsilon \tag{5}$$

substituting (5) into (40), one obtains

$$\hat{u} = UQ^{-1}Hu + UQ^{-1}\epsilon \tag{41}$$

Recalling that $E\epsilon = 0$, one has

$$E\hat{u} = UQ^{-1}Hu \tag{42}$$

Taking the transpose of both sides of (40), one observes

$$\hat{u}^T = y^TQ^{-1}U^T$$

which can be simplified into

$$\hat{u}^T = (Hu + \epsilon)^TQ^{-1}U^T = (u^TH^T + \epsilon^T)Q^{-1}U^T \tag{43}$$

Hence taking the expected value of both sides of (43), one reaches

$$E\hat{u}^T = u^T H^T Q^{-1} U^T \tag{44}$$

The formula for ψ derived from the definition (see p. 16) is recalled here

$$\psi = E(\hat{u}\hat{u}^T) - (E\hat{u})(E\hat{u}^T) \tag{45}$$

Substituting (41), (42), and (44) into (45) and simplifying it, one has

$$\begin{aligned}\psi &= E[(UQ^{-1}Hu + UQ^{-1}\epsilon)(UQ^{-1}Hu + UQ^{-1}\epsilon)^T] - (UQ^{-1}Hu)(u^T H^T Q^{-1} U^T) \\ &= UQ^{-1}E(\epsilon\epsilon^T)Q^{-1}U^T\end{aligned} \tag{46}$$

Recalling that one of the assumptions of the linear model is

$$E(\epsilon\epsilon^T) = Q$$

and substituting it into (46), one finally arrives at

$$\psi = UQ^{-1}U^T$$

APPENDIX D

FORMULAS FOR LEAST SQUARE ESTIMATORS AND VARIANCE COVARIANCE MATRICES FOR FOUR FITTING PROCEDURES

The formulas for the least square estimators, which are the solutions of the four fitting procedures, and the expressions for the variance covariance matrices, which can give the formulas for the standard deviations of the least square estimators, are listed here. The matrix notation is used for conciseness.

1. Overdetermined Case

   (i) Procedure no. 1, the standard least square, no constraint fit (see p. 7), finds x which minimizes $(Hx-y)^T Q^{-1}(Hx-y)$. The solution is $x = (H^T Q^{-1} H)^{-1} H^T Q^{-1} y$, and the variance covariance matrix is $\psi = (H^T Q^{-1} H)^{-1}$.

   (ii) Procedure no. 2, the ellipsoidal fit (see p. 7), finds x which minimizes $(Hx-y)^T Q^{-1}(Hx-y)$ subject to $x^T W^{-1} x \leq 1.0$. The solution is $x = (H^T Q^{-1} H + \lambda W^{-1})^{-1} H^T Q^{-1} y$, and the variance covariance matrix is $\psi = (Q^{-1/2} HU)^T (Q^{-1/2} HU)$, where $U = [H^T Q^{-1} H + \lambda W^{-1}]^{-1}$.

   (iii) Procedure no. 3, the combined fit (see p. 8), finds x which minimizes $(Hx-y)^T Q^{-1}(Hx-y) + x^T P^{-1} x$. The solution is $x = (H^T Q^{-1} H + P^{-1})^{-1} H^T Q^{-1} y$, and the variance covariance matrix is $\psi = (Q^{-1/2} HU)^T (Q^{-1/2} HU)$, where $U = [H^T Q^{-1} H + P^{-1}]^{-1}$.

(iv) Procedure no. 4, the fixed square fit (see p. 8), finds x which minimizes $x^T P^{-1} x$ subject to $\frac{1}{N}[(Hx-y)^T Q^{-1}(Hx-y)] = 1.0$. The solution is $x = [H^T Q^{-1} H + \frac{P^{-1}}{\lambda}]^{-1} H^T Q^{-1} y$, and the variance covariance matrix is $\psi = (Q^{-1/2}HU)^T (Q^{-1/2}HU)$, where $U = [H^T Q^{-1} H + \frac{P^{-1}}{\lambda}]^{-1}$.

2. Underdetermined Case

To find a unique solution for the underdetermined case of the standard least square fit, one can define the following procedure (see p. 18). The procedure finds the x which, among all the x that minimize $(Hx-y)^T Q^{-1}(Hx-y)$, also minimizes $x^T P^{-1} x$; there are two forms of solution depending on the availability of computer storage.

The form of solution which takes less memory storage is $x = P^{1/2}[(HP^{1/2})^T Q^{-1}(HP^{1/2})]^+ (HP^{1/2})^T Q^{-1} y$, and the variance covariance matrix is $\psi = UQ^{-1}U^T$, where $U = P^{1/2}[(HP^{1/2})^T Q^{-1}(HP^{1/2})]^+ (HP^{1/2})^T$.

APPENDIX E

RELATION OF THE PSEUDOINVERSE OF A MATRIX WITH THAT OF A SYMMETRIC MATRIX[27]

The following is the proof of a formula which enables any user to transform the pseudoinverse of a non-symmetric matrix into the pseudoinverse of a symmetric matrix; this has the definite advantage of reducing the computer storage allocated to the pseudoinverse routine in the event that the matrix which needs to be pseudoinversed is highly underdetermined, that is the number of the columns is much larger than that of the rows.

Show that for any matrix H,

$$H^{+} = (H^{T}H)^{+}H^{T} \tag{47}$$

Proof: Let one first use a lemma which will be proved later;

for any matrix H, $(H^{T}H)^{+} = H^{+}(H^{T})^{+}$ (48)

Substituting (48) into the left hand side of (47), one can show

$$(H^{T}H)^{+}H^{T} = H^{+}(H^{T})^{+}H^{T} = H^{+}(H^{+})^{T}H^{T} = H^{+}(HH^{+})^{T} = H^{+}HH^{+} = H^{+} \qquad \text{Q.E.D.}$$

Lemma: Show that for any matrix H

$$(H^{T}H)^{+} = H^{+}(H^{T})^{+} \tag{48}$$

Proof: From the definition of the pseudoinverse of H^TH, the four relations below must hold.

$$(H^TH)(H^TH)^+ = ((H^TH)(H^TH)^+)^T \tag{49}$$

$$(H^TH)^+(H^TH) = ((H^TH)^+(H^TH))^T \tag{50}$$

$$(H^TH)(H^TH)^+(H^TH) = (H^TH) \tag{51}$$

and

$$(H^TH)^+(H^TH)(H^TH)^+ = (H^TH)^+ \tag{52}$$

If one substitutes (48) into these four relations and can show $H^+(H^T)^+$ satisfies them, the proof is completed.

Substituting (48) into the left hand side of (49), one sees that

$$((H^TH)H^+(H^T)^+)^T = H^+(H^+)^T(H^TH) = H^+HH^+H = H^+H$$

The right hand side of (49) can be simplified into

$$(H^TH)(H^+(H^T)^+) = H^T(H^T)^+H^T(H^T)^+ = (H^T(H^T)^+)^T(H^T(H^T)^+)^T = H^+HH^+H = H^+H$$

Thus the right hand side of (49) is equal to the left hand side of (49).

Substituting (48) into (50) and using R.H.S. and L.H.S. to denote the right and left hand sides, respectively, one observes that

$$\text{R.H.S. of (50) is } H^+(H^T)^+H^TH = H^+((H^T)^+H^T)^TH = H^+HH^+H = H^+H$$

L.H.S. of (50) is $(H^{+}(H^{T})^{+}H^{T}H)^{T} = H^{T}HH^{+}(H^{+})^{T} = H^{T}(H^{T})^{+}H^{T}(H^{+})^{T}$

$= H^{T}(H^{+})^{T} = H^{+}H$

Substituting (48) into (51), one finds that

L.H.S. of (51) is $(H^{T}H)H^{+}(H^{T})^{+}(H^{T}H) = H^{T}(H^{T})^{+}H^{T}(H^{T})^{+}H^{T}H$

$= H^{T}(H^{T})^{+}H^{T}H = H^{T}H =$ R.H.S. of (51).

Substituting (48) into (52), one obtains

L.H.S of (52) is $H^{+}(H^{T})^{+}H^{T}HH^{+}(H^{T})^{+} = H^{+}HH^{+}HH^{+}(H^{T})^{+} = H^{+}HH^{+}(H^{T})^{+}$

$= H^{+}(H^{T})^{+} =$ R.H.S. of (52).

Q.E.D.

APPENDIX F

FLOWCHARTS OF FITTING PROGRAMS

An initial attempt was made to develop a computer code which would include all four fitting procedures. However, in the tedious process of debugging and alterations, experience led to the conclusion that for the investigations one wishes to perform it would be much simpler to write a program for each scheme separately. Finally, upon the discovery of the similar logic involved in procedures no. 1 and no. 3, their programs were combined into one main program which was called PRO3.MAIN2 and their corresponding subroutines were stored accordingly in the file PRO3. As for procedures no. 2 and no. 4, their main programs and subroutines can be retrieved from files PRO2 and PRO4, respectively. In their simplified flowcharts, the PRO2.MAIN2 and the PRO4.MAIN2 seem to have a similar sequence of reasoning; however, due to the difference between their constraints, each fitting procedure contains a different method for determining the La Grange multiplier.

As a final note, all the subroutines having the same element name in the above mentioned three files are identical. This was achieved by first developing working modules for every specific calculation, and later on stacking them together in consistence with the logic of each particular fitting scheme.

The flowcharts follow as Figures 17, 18, and 19.

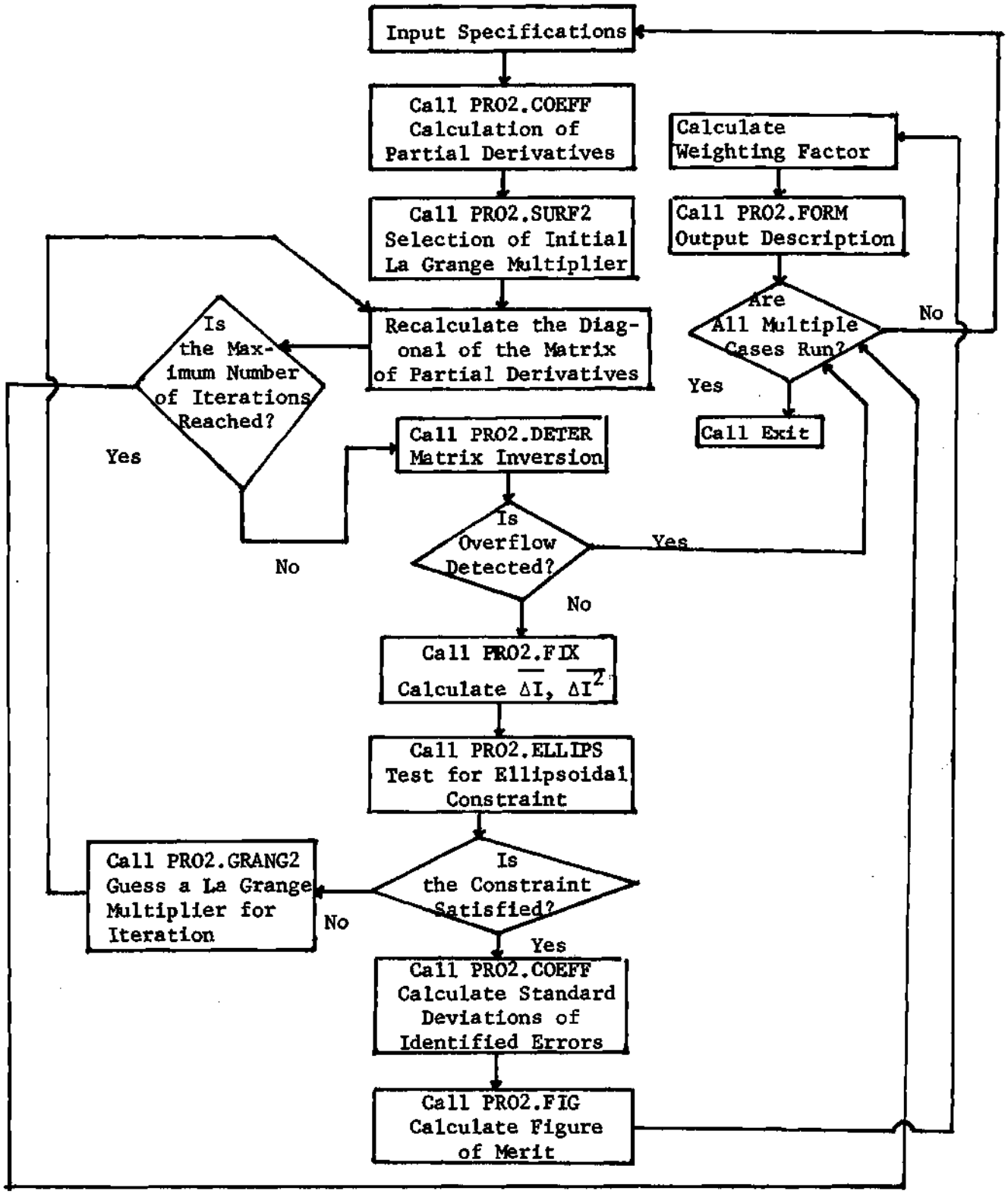


Figure 17. The Flowchart of PRO2.MAIN2

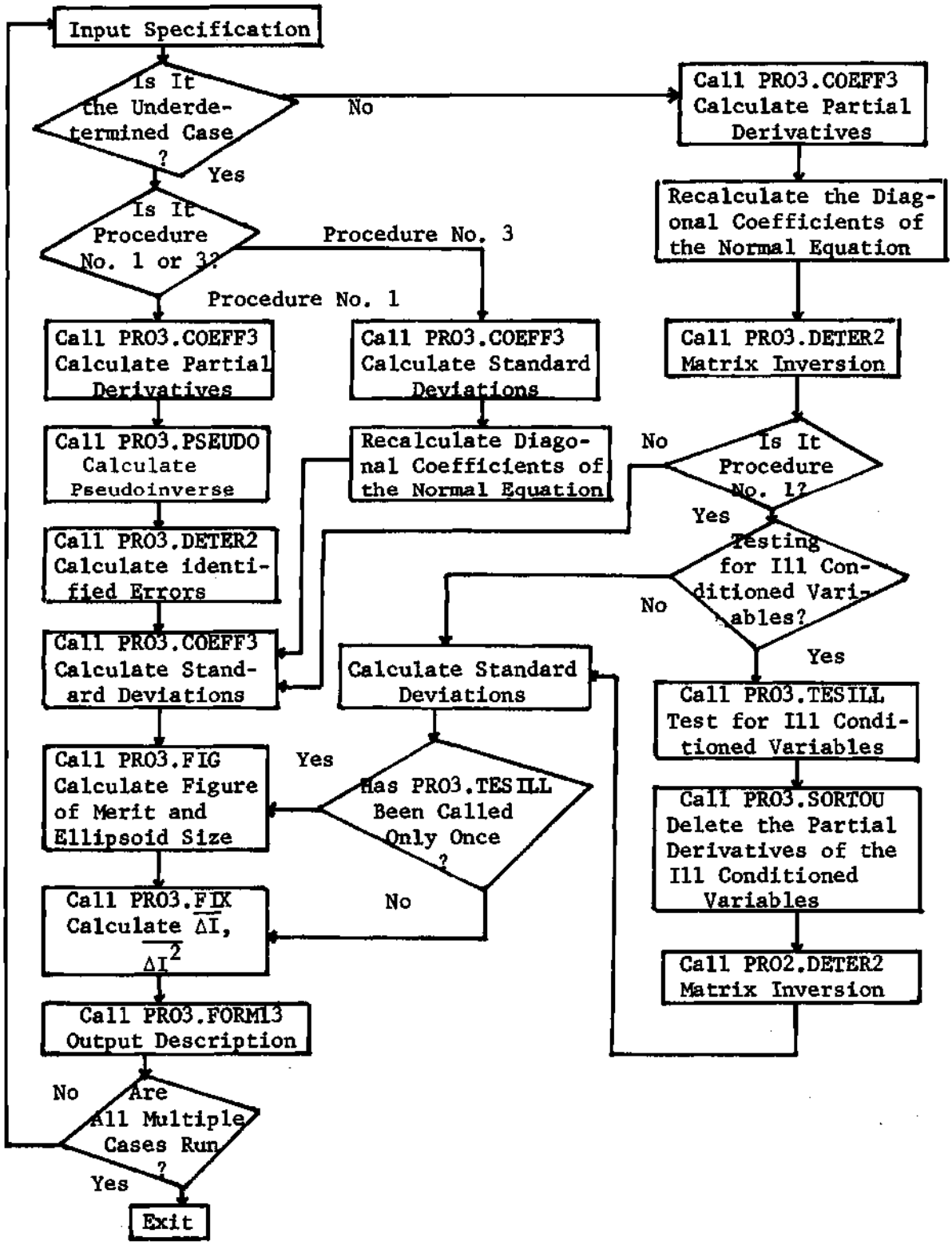


Figure 18. The Flowchart of PRO3.MAIN2

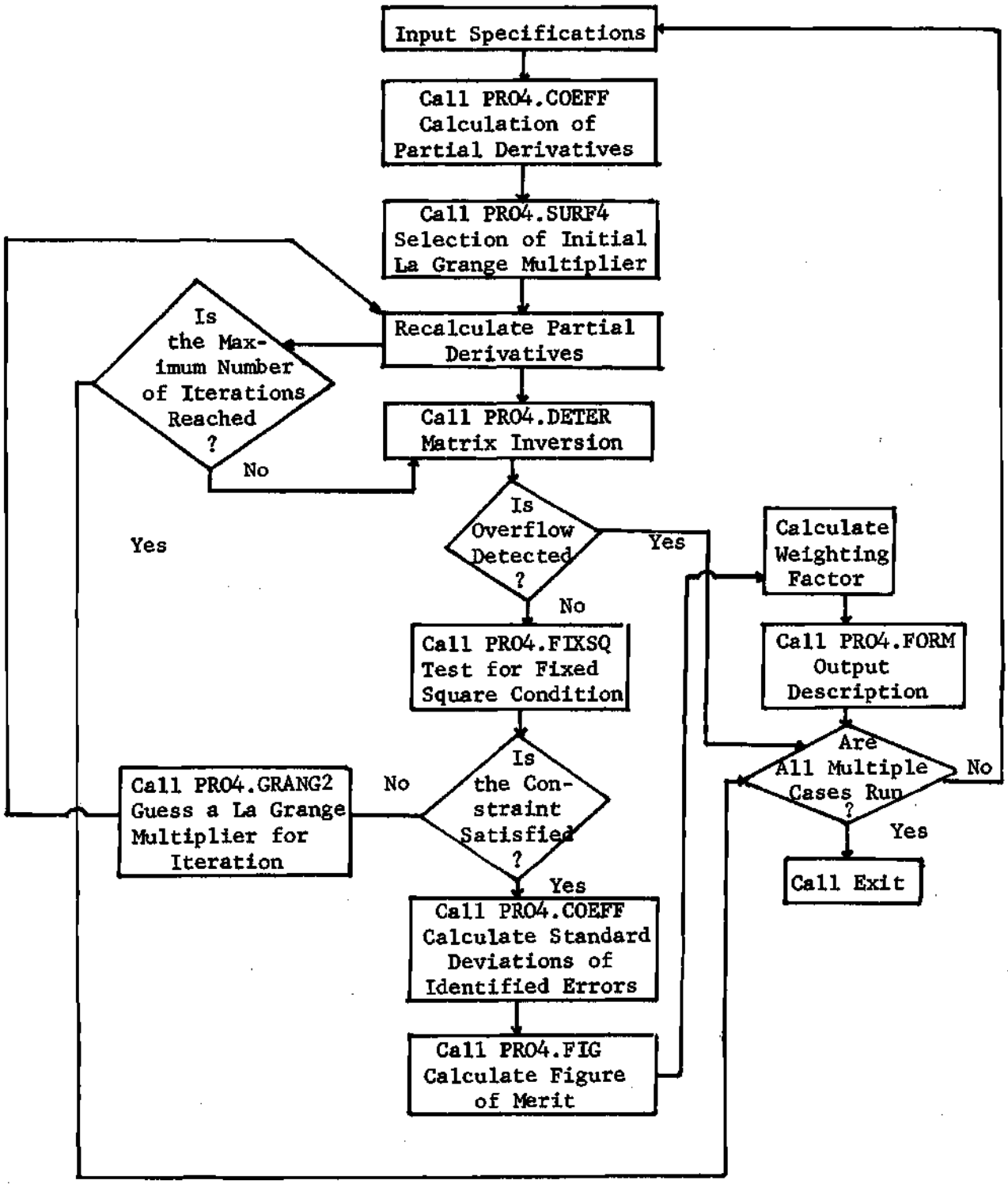


Figure 19. The Flowchart of PRO4.MAIN2

APPENDIX G

TABLES OF RESULTS FROM FITTING PROCEDURES

All four fitting programs contain the subroutine FORM which prints out the results of any error identification in a tabulated form for easy reference.

The following is a brief description of the terminologies in a typical computer printout.

ASD designates $\overline{\Delta I^2}$ whereas AD designates $\overline{\Delta I}$. The error in either k or the reaction rate ratio actually refers to the standard deviation of the statistical error in the mentioned integral data. FM denotes the overall figure of merit. The rest of the printout is self explanatory.

Table 13 represents a typical case of an ellipsoidal fit which uses the optimal beta of 2.5, 22 unknowns, and 27 integral data. This case shows that the optimal beta gives good results for error identification for many important cross sections.

Tables 14 and 15 contain the results from two highly overdetermined cases of the combined fit. As expected, the error identification improves as the degree of overdeterminedness increases.

As the standard deviation of the statistical error of the integral data decreases, the error identification improves tremendously. This can be seen by comparing Table 16 with Table 17.

With exceedingly large systematic errors of -.02 for the k values and -.2 for the reaction rate ratios, the error identification for the

ellipsoidal fit which uses the optimal beta of 2.5, 22 unknowns, and 27 integral data deteriorates considerably. One can compare the results for this case which is shown in Table 18 with results in Table 13, which is the same fit but without any systematic error.

Tables 19, 20, and 21 contain the results for three highly overdetermined cases of the standard least square fit. As discussed previously, the error identification using this fit improves only if the degree of overdeterminedness increases drastically.

Even though Tables 22 and 23 are both highly underdetermined, one still observes that the case with the k values and the reaction rate ratios yields better error identification for several, very important cross sections than the case with reaction rate ratios only. This effect has been discussed in the previous section.

As has been discussed previously, the figures of merit obtained in this study are much higher than those in the one group work.[22] This is mainly due to the fact that this study employs a more systematic method of introducing errors; as a result more small errors are introduced in this study than in the previous one group work.[22]

Since a value of 0.1 S^{σ} is used for the definition of a small introduced error, it is difficult for a fitting procedure to identify such a small introduced error. Although many identified errors which correspond to the small introduced errors do not fall within 0.1 S^{σ} of the small introduced errors, their individual figures of merit (1.0 in this case) are still included in the calculation of the overall figure of merit. However, in the figure of merit defined in the previous one group study,[22]

the worst half of the identified errors would have been eliminated, and the remaining half would have consisted mainly of the large identified errors which were related to the large introduced errors. Therefore, the figures of merit in the previous one group study[22] are much better than those in this study.

As shown in Tables 22 and 23, many introduced errors are quite small and have not been identified by the fitting procedure. This is one of the reasons why the overall figures of merit for these cases are not that good. Another reason is that these cases are highly underdetermined; the error identification is expected to be less meaningful than those overdetermined cases. However, comparing Table 22 with Table 23, one can still see the error identification of some important cross sections for the mixture of the k and reaction rate ratios is better than for the reaction rate ratios only.

Table 13. An Ellipsoidal Fit with the Empirical Beta of 2.5 BLACK.3D8T5-3G-FE with 3 Groups, 22 Unknowns, 9 k Values with S^I = .001, 18 Reaction Rate Ratios with S^I = .03

********** 3 GROUP: ELLIPSOIDAL CONSTRAINT **********
WITH GAMMA = .23062+00
ERROR IN K = .10000-02 SYSTEM ERROR = .00000
IN ASBLY 21,22,23,24,25,26,27,29,30,
ERROR IN U238 CAPT/U235 FIS = .30000-01 SYSTEM ERROR = .00000
IN ASBLY 21,22,23,24,25,26,27,29,30,
ERROR IN U238 FIS/U235 FIS = .30000-01 SYSTEM ERROR = .00000
IN ASBLY 21,22,23,24,25,26,27,29,30,
BETA = .25000+01 FM = .59920+00 ASD = .75888+00 AD =-.14847-02

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
U235	SGCAP1	.50000+01	-.12810+01	-.22843-01	.47026-01
U238	SGCAP1	.10000+02	.12834+02	-.60077+01	.24610+01
FE	SGCAP1	.20000+02	-.42810+02	-.10561+01	.24863+01
U235	SGFIS1	.30000+01	-.45835+01	-.40645+00	.68024+00
U238	SGFIS1	.30000+01	.36410+00	.11914+00	.11974+01
U235	SGTR-1	.20000+02	-.38580+01	-.56886+01	.52534+01
U238	SGTR-1	.20000+02	-.94126+01	-.16081+02	.12113+02
FE	SGTR-1	.20000+02	.57636+01	-.46789+01	.14028+02
U235	SGCAP2	.50000+01	-.45824+01	-.20416+01	.17467+01
U238	SGCAP2	.10000+02	-.84593+00	-.20255+01	.20714+01
FE	SGCAP2	.20000+02	-.43235+01	-.34705+01	.12321+02
U235	SGFIS2	.30000+01	.20664+01	.32756+00	.17386+01
U235	SGTR-2	.15000+02	-.55458+01	.33726+00	.65617+01
U238	SGTR-2	.20000+02	.12166+02	.14104+02	.78922+01
FE	SGTR-2	.20000+02	-.27542+02	-.21432+02	.77759+01
U235	SGCAP3	.50000+01	-.66301+01	-.50152+01	.30597+01
U238	SGCAP3	.10000+02	.76163+01	.62172+01	.36486+01
FE	SGCAP3	.10000+02	-.11418+01	.53377+01	.66419+01
U235	SGFIS3	.30000+01	-.28604+01	-.24475+01	.20223+01
U235	SGTR-3	.10000+02	.24379+01	.11735+01	.12804+01
U238	SGTR-3	.20000+02	-.10448+02	-.37061+01	.13614+02
FE	SGTR-3	.10000+02	-.25208+01	.62344+01	.45606+01

Table 14. A Combined Fit to Study the Influence of the Degree of Overdeterminedness BLACK.3D8T9-2G with 2 Groups, 10 Unknowns, 10 k Values, and 20 Reaction Rate Ratios

********** 2 GROUP: COMBINED FIT **********

WITH GAMMA = .10000+01

ERROR IN K = .10000-02 SYSTEM ERROR = .00000

IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,

ERROR IN U^{238} CAPT/PU^{239} FIS = .30000-01 SYSTEM ERROR = .00000

IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,

ERROR IN U^{238} FIS/PU^{239} FIS = .30000-01 SYSTEM ERROR = .00000

IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,

BETA = .28221+01 FM = .59245+00 ASD = .80802+00 AD =-.97961-01

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	S_GCAP1	.50000+01	-.12810+01	.65870+00	.13946+00
U238	S_GCAP1	.10000+02	.12834+02	.70812+01	.31115+01
PU239	S_GFIS1	.30000+01	-.64215+01	-.68120+01	.95982+00
PU239	S_GTR-1	.20000+02	-.30557+02	-.18517+02	.82300+01
U238	S_GTR-1	.20000+02	.24273+01	.10778+01	.18789+01
PU239	S_GCAP2	.50000+01	-.96450+00	-.50213+01	.20394+01
U238	S_GCAP2	.10000+02	-.47063+01	-.49910+01	.12009+01
PU239	S_GFIS2	.30000+01	.86454+00	-.78551+00	.83276+00
PU239	S_GTR-2	.10000+02	-.91648+01	-.35842+00	.17072+01
U238	S_GTR-2	.10000+02	-.84593+00	-.31953+01	.39634+01

Table 15. A Combined Fit to Study the Influence of the Degree of Overdeterminedness BLACK.3D8T9-2G-1 with 2 Groups, 10 Unknowns, 20 k Values, and 40 Reaction Rate Ratios

********** 2 GROUP: COMBINED FIT **********
WITH GAMMA = .10000+01
ERROR IN K = .10000-02 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,

ERROR IN U238 CAPT/PU239 FIS = .30000-01 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,

ERROR IN U238 FIS/PU239 FIS = .30000-01 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,

BETA = .28477+01 FM = .46377+00 ASD = .69922+00 AD =-.19742-01

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAP1	.50000+01	-.12810+01	.53898+00	.16051+00
U238	SGCAP1	.10000+02	.12834+02	.10221+02	.32677+01
PU239	SGFIS1	.30000+01	-.64215+01	-.64535+01	.88788+00
PU239	SGTR-1	.20000+02	-.30557+02	-.21978+02	.79887+01
U238	SGTR-1	.20000+02	.24273+01	.12636+01	.17116+01
PU239	SGCAP2	.50000+01	-.96450+00	-.43973+01	.19563+01
U238	SGCAP2	.10000+02	-.47063+01	-.57302+01	.10432+01
PU239	SGFIS2	.30000+01	.86454+00	-.87200+00	.79246+00
PU239	SGTR-2	.10000+02	-.91648+01	-.63389+00	.24764+01
U238	SGTR-2	.10000+02	-.84593+00	-.15402+01	.36111+01

Table 16. A Combined Fit to Study the Influence of a Small Statistical Error of Experimental Integral Data BLACK.DK09CF-4G-FE with 4 Groups, 30 Unknowns, 9 k Values with S^I = .001, and 9 Reaction Rate Ratios with S^I = .03

********** 4 GROUP: COMBINED FIT **********
WITH GAMMA = .10000+01
ERROR IN K = .10000-02 SYSTEM ERROR = .00000
IN ASBLY 31,32,33,34,35,36,37,39,40,
ERROR IN PU240 CAPT/PU239 FIS = .30000-01 SYSTEM ERROR = .00000
IN ASBLY 31,32,33,34,35,36,37,39,40,
BETA = .24584+01 FM = .81457+00 ASD = .68604+00 AD =-.34285-01

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAP1	.50000+01	-.12810+01	.30641-04	.38604-02
PU240	SGCAP1	.10000+02	.12834+02	-.13945+00	.96123-01
FE	SGCAP1	.20000+02	-.42810+02	-.26592+00	.48735+00
PU239	SGFIS1	.30000+01	-.45835+01	-.10241+00	.29692+00
PU240	SGFIS1	.30000+01	.36410+00	-.45716-01	.54492+00
PU239	SGTR-1	.20000+02	-.38580+01	-.12559+01	.33534+01
PU240	SGTR-1	.20000+02	-.94126+01	-.40174-01	.15879+01
FE	SGTR-1	.20000+02	.57636+01	-.93081+01	.59037+01
PU239	SGCAP2	.50000+01	-.45824+01	-.79084-01	.55469-01
PU240	SGCAP2	.10000+02	-.84593+00	-.63598+00	.19798+01
FE	SGCAP2	.20000+02	-.43235+01	-.44117+00	.19093+01
PU239	SGFIS2	.30000+01	.20664+01	.11798+01	.71507+00
PU240	SGFIS2	.30000+01	-.11092+01	.35866+00	.76026+00
PU239	SGTR-2	.20000+02	.12166+02	-.33325+01	.60743+01
PU240	SGTR-2	.20000+02	-.27542+02	.62924+00	.41534+01
FE	SGTR-2	.20000+02	-.26520+02	-.30499+02	.54057+01
PU239	SGCAP3	.50000+01	.38082+01	-.15198+00	.40569+00
PU240	SGCAP3	.10000+02	-.11418+01	-.29790+01	.26298+01
FE	SGCAP3	.20000+02	-.19069+02	-.21196+01	.29623+01
PU239	SGFIS3	.30000+01	.73138+00	.12528+01	.81578+00

Table 16. Concluded

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU240	SGFIS3	.30000+01	-.15672+01	.14056-01	.43641-01
PU239	SGTR-3	.10000+02	-.25208+01	-.95723+00	.10176+01
PU240	SGTR-3	.20000+02	.10958+01	-.19554+01	.30768+01
FE	SGTR-3	.20000+02	-.12036+02	.50359+01	.71191+01
PU239	SGCAP4	.50000+01	-.11093+01	-.24598+01	.84858+00
PU240	SGCAP4	.10000+02	-.80538+01	-.10966+02	.25129+01
FE	SGCAP4	.50000+01	.82382+01	-.25455+00	.91799+00
PU239	SGFIS4	.50000+01	.10686+02	.60974+01	.12161+01
PU239	SGTR-4	.10000+02	-.13367+02	-.39698-01	.32179+00
PU240	SGTR-4	.20000+02	.24518+02	-.83781+00	.64845+00

Table 17. A Combined Fit to Study the Influence of an Extremely Small Statistical Error of Experimental Integral Data BLACK.DK09CF-4G-FE with 4 Groups, 30 Unknowns, 9 k Values with $S^I = 10^{-6}$, and 9 Reaction Rate Ratios with $S^I = 3 \times 10^{-5}$

```
********************** 4 GROUP: COMBINED FIT **************************
                        WITH GAMMA = .10000+01
ERROR IN K = .10000-05      SYSTEM ERROR = .00000
IN ASBLY 31,32,33,34,35,36,37,39,40,
ERROR IN PU240 CAPT/PU239 FIS = .30000-04   SYSTEM ERROR = .00000
IN ASBLY 31,32,33,34,35,36,37,39,40,
BETA = .40714+01  FM = .50760+00  ASD = .42339-02  AD = .15154-05
```

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAP1	.50000+01	-.12810+01	.91606-02	.26313-02
PU241	SGCAP1	.10000+02	.12834+02	.46637+01	.14732+01
FE	SGCAP1	.20000+02	-.42810+02	-.88396+01	.75554+00
PU239	SGFIS1	.30000+01	-.45835+01	-.35067+01	.58982+00
PU241	SGFIS1	.30000+01	.36410+00	.64486+00	.35445+00
PU239	SGTR-1	.20000+02	-.38580+01	-.13489+02	.38593+01
PU241	SGTR-1	.20000+02	-.94126+01	-.19449+02	.12980+01
FE	SGTR-1	.20000+02	.57636+01	.57181+01	.11266+01
PU239	SGCAP2	.50000+01	-.45824+01	-.71017+00	.10497+00
PU241	SGCAP2	.10000+02	-.84593+00	-.26148+00	.16166+00
FE	SGCAP2	.20000+02	-.43235+01	-.20080+02	.16055+01
PU239	SGFIS2	.30000+01	.20664+01	.15166+01	.22471+00
PU241	SGFIS2	.30000+01	-.11092+01	-.44535+00	.47171+00
PU239	SGTR-2	.20000+02	.12166+02	.18443+02	.28431+01
PU241	SGTR-2	.20000+02	-.27542+02	-.16042+02	.18252+01
FE	SGTR-2	.20000+02	-.26520+02	-.26387+02	.34849+00
PU239	SGCAP3	.50000+01	.38082+01	-.28794+01	.30580+00
PU241	SGCAP3	.10000+02	-.11418+01	-.16541+01	.90044-01
FE	SGCAP3	.20000+02	-.19069+02	-.16470+02	.28050+01

Table 17. Concluded

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGFIS3	.30000+01	.73138+00	.30366+00	.17182+00
PU240	SGFIS3	.30000+01	-.15672+01	.60815-01	.49522-01
PU239	SGTR-3	.10000+02	-.25208+01	-.44053+01	.12291+01
PU241	SGTR-3	.20000+02	.10958+01	-.12767+02	.15530+01
FE	SGTR-3	.20000+02	-.12036+02	-.13051+02	.41584+00
PU239	SGCAP4	.50000+01	-.11093+01	-.92639+00	.30916+00
PU241	SGCAP4	.10000+02	-.80538+01	-.81619+01	.64779-01
FE	SGCAP4	.50000+01	.82382+01	.61551+01	.39429+00
PU239	SGFIS4	.50000+01	.10686+02	.10395+02	.16884+00
PU239	SGTR-4	.10000+02	-.13367+02	-.15155+01	.20643+01
PU240	SGTR-4	.20000+02	.24518+02	-.31964+01	.46253+01

Table 18. An Ellipsoidal Fit to Study the Influence of the Systematic Errors BLACK.3D8T5-3G-FE with 3 Groups, 22 Unknowns, 9 k Values, and 18 Reaction Rate Ratios

```
**************** 3 GROUP: ELLIPSOIDAL CONSTRAINT ****************
                        WITH GAMMA = .45844+02
ERROR IN K = .10000-02      SYSTEM ERROR =-.20000-01
IN ASBLY 21,22,23,24,25,26,27,29,30,
ERROR IN U238 CAPT/U235 FIS = .30000-01   SYSTEM ERROR =-.20000+00
IN ASBLY 21,22,23,24,25,26,27,29,30,
ERROR IN U238 FIS/U235 FIS = .30000-01   SYSTEM ERROR =-.20000+00
IN ASBLY 21,22,23,24,25,26,27,29,30,
BETA = .25000+01  FM = .83097+00  ASD = .19952+02  AD =-.36627+01
```

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
U235	SGCAP1	.50000+01	-.12810+01	.53776-01	.17875-02
U238	SGCAP1	.10000+02	.12834+02	.12726+00	.55207-01
FE	SGCAP1	.20000+02	-.42810+02	.62689+00	.45037-01
U235	SGFIS1	.30000+01	-.45835+01	-.43034+00	.17668-01
U238	SGFIS1	.30000+01	.36410+00	-.47664+01	.17506+00
U235	SGTR-1	.20000+02	-.38580+01	-.73961+00	.15912+00
U238	SGTR-1	.20000+02	-.94126+01	-.35233+01	.69050+00
FE	SGTR-1	.20000+02	.57636+01	-.11293+02	.59302+00
U235	SGCAP2	.50000+01	-.45824+01	.10946+01	.52709-01
U238	SGCAP2	.10000+02	-.84593+00	-.47285+01	.40858+00
FE	SGCAP2	.20000+02	-.43235+01	.20532+01	.26098+00
U235	SGFIS2	.30000+01	.20664+01	-.31911+01	.98292-01
U235	SGTR-2	.15000+02	-.55458+01	-.32233+00	.17597+00
U238	SGTR-2	.20000+02	.12166+02	-.97093+00	.10232+01

Table 18. Concluded

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
FE	SGTR-2	.20000+02	-.27542+02	-.14327+02	.64521+00
U235	SGCAP3	.50000+01	-.66301+01	.25735+01	.17881+00
U238	SGCAP3	.10000+02	.76163+01	.15155+01	.61021+00
FE	SGCAP3	.10000+02	-.11418+01	.75784+00	.19678+00
U235	SGFIS3	.30000+01	-.28604+01	-.31567+01	.12639+00
U235	SGTR-3	.10000+02	.24379+01	-.16200+00	.21017-01
U238	SGTR-3	.20000+02	-.10448+02	-.19294+01	.25671+00
FE	SGTR-3	.10000+02	-.25208+01	-.96347+00	.14630+00

Table 19. A Standard Least Square Fit to Study the Influence of the Degree of Overdeterminedness BLACK.3D8T9-2G with 2 Groups, 10 Unknowns, 10 k Values, and 20 Reaction Rate Ratios

********** 2 GROUP: NO CONSTRAINT **********
0 VARIABLES ELIMINATED
ERROR IN K = .30000-02 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,
ERROR IN U^{238} CAPT/PU^{239} FIS = .50000-01 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,
ERROR IN U^{238} FIS/PU^{239} FIS = .50000-01 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,
BETA = .57848+02 FM = .95572+00 ASD = .69095+00 AD =-.33908-01

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAP1	.50000+01	-.12810+01	.17015+03	.79124+03
U238	SGCAP1	.10000+02	.12834+02	.21210+02	.27629+02
PU239	SGFIS1	.30000+01	-.64215+01	.26646+01	.31886+02
PU239	SGTR-1	.20000+02	-.30557+02	-.30340+03	.17889+03
U238	SGTR-1	.20000+02	.24273+01	.45176+02	.27027+02
PU239	SGCAP2	.50000+01	-.96450+00	.59214+01	.15015+02
U238	SGCAP2	.10000+02	-.47063+01	-.89636+01	.56641+01
PU239	SGFIS2	.30000+01	.86454+00	-.23192+01	.34446+01
PU239	SGTR-2	.10000+02	-.91648+01	.43459+03	.26312+03
U238	SGTR-2	.10000+02	-.84593+00	-.75069+02	.50483+02

Table 20. A Standard Least Square Fit to Study the Influence of the Degree of Overdeterminedness BLACK.3D8T9-2G-1 with 2 Groups, 10 Unknowns, 20 k Values, and 40 Reaction Rate Ratios

********** 2 GROUP: NO CONSTRAINT **********
0 VARIABLES ELIMINATED
ERROR IN K = .30000-02 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,

ERROR IN U238 CAPT/PU239 FIS = .50000-01 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,

ERROR IN U238 FIS/PU239 FIS = .50000-01 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,

BETA = .15618+02 FM = .89650+00 ASD = .67005+00 AD = .67687-02

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAP1	.50000+01	-.12810+01	-.23683+01	.43455+03
U238	SGCAP1	.10000+02	.12834+02	.22149+02	.15422+02
PU239	SGFIS1	.30000+01	-.64215+01	-.39144+01	.15934+02
PU239	SGTR-1	.20000+02	-.30557+02	-.11417+03	.10004+03
U238	SGTR-1	.20000+02	.24273+01	.17965+02	.15533+02
PU239	SGCAP2	.50000+01	-.96450+00	-.33655+01	.84710+01
U238	SGCAP2	.10000+02	-.47063+01	-.96361+01	.35443+01
PU239	SGFIS2	.30000+01	.86454+00	-.27028+01	.23644+01
PU239	SGTR-2	.10000+02	-.91648+01	.13861+03	.13277+03
U238	SGTR-2	.10000+02	-.84593+00	-.30588+02	.28832+02

Table 21. A Standard Least Square Fit to Study the Influence of the Degree of Overdeterminedness BLACK.3D8T9-2G-2 with 2 Groups, 10 Unknowns, 40 k Values, and 80 Reaction Rate Ratios

********** 2 GROUP: NO CONSTRAINT **********
0 VARIABLES ELIMINATED
ERROR IN K = .30000-02 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,
31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,
ERROR IN U238 CAPT/PU239 FIS = .50000-01 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,
31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,
ERROR IN U238 FIS/PU239 FIS = .50000-01 SYSTEM ERROR = .00000
IN ASBLY 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18,19,20,
31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,
BETA = .28699+02 FM = .71953+00 ASD = .81619+00 AD = .63721-02

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAP1	.50000+01	-.12810+01	.14282+03	.27563+03
U238	SGCAP1	.10000+02	.12834+02	.18946+02	.95170+01
PU239	SGFIS1	.50000+01	-.64215+01	-.11256+01	.97550+01
PU239	SGTR-1	.20000+02	-.30557+02	-.29196+02	.56636+02
U238	SGTR-1	.20000+02	.24273+01	.58565+01	.95057+01
PU239	SGCAP2	.50000+01	-.96450+00	.12680+00	.41862+01
U238	SGCAP2	.10000+02	-.47063+01	-.64328+01	.22810+01
PU239	SGFIS2	.30000+01	.86454+00	.40454+00	.14767+01
PU239	SGTR-2	.10000+02	-.91648+01	-.44985+00	.68104+02
U238	SGTR-2	.10000+02	-.84593+00	-.11624+02	.17647+02

Table 22. An Ellipsoidal Fit to Study the Influence of Different Types of Integral Data, BLACK.2DOT9-3G-FE with 3 Groups, 24 Unknowns, 18 Reaction Rate Ratios

```
****************** 3 GROUP ELLIPSOIDAL CONSTRAINT ******************
                        .IPU GAMMA = .47437-01
ERROR IN PU240 CAPT/PU239 FIS = .70000-01   SYSTEM ERROR = .00000
IN ASSLY 31,32,33,34,35,36,37,38,40,
ERROR IN PU240 FIS/PU239 FIS = .70000-01   SYSTEM ERROR = .00000
IN ASSLY 31,32,33,34,35,36,37,38,40,
DELTA = .25000+01  FM = .64893+00  ASU = .66594+00  AD =-.47115-02
```

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAP1	.50000+01	-.12810+01	.42178-02	.70269-02
PU240	SGCAP1	.10000+02	.12334+02	-.21567+01	.22647+01
FE	SGCAP1	.20000+02	-.42810+02	-.06376-01	.21571+00
PU239	SGFIS1	.30000+01	-.45835+01	-.07147+00	.87765+00
PU240	SGFIS1	.30000+01	.36410+00	-.23168+01	.33940+01
PU239	SGTR-1	.20000+02	-.30580+01	-.12235+01	.18015+01
PU240	SGTR-1	.20000+02	-.94126+01	-.05867+00	.56406+00
FE	SGTR-1	.20000+02	.57636+01	-.03637+01	.64345+01
PU239	SGCAP2	.50000+01	-.45924+01	-.16184+00	.37309+00
PU240	SGCAP2	.10000+02	-.84593+00	-.18785+01	.72804+01
FE	SGCAP2	.20000+02	-.43235+01	.24569+01	.42688+01
PU239	SGFIS2	.30000+01	.20664+01	-.06161+01	.26913+01
PU240	SGFIS2	.30000+01	-.11092+01	.14173+01	.22504+01
PU239	SGTR-2	.15000+02	.91247+01	.40860+01	.60348+01
PU240	SGTR-2	.20000+02	-.27542+02	.19136+01	.39009+01
FE	SGTR-2	.20000+02	-.26520+02	.38673+01	.36497+02

Table 22. Concluded

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAPS	.50000+01	.38082+01	.29845+01	.44150+01
PU240	SGCAPS	.10000+02	-.11418+01	-.53022+01	.64046+01
FE	SGCAPS	.10000+02	-.95346+01	.25786+01	.65866+01
PU239	SGFISS	.50000+01	.12190+01	.01093+01	.60925+01
PU240	SGFISS	.30000+01	-.15672+01	.03658-02	.48555-01
PU239	SGTR-S	.10000+02	-.25208+01	-.01899+00	.83790+00
PU240	SGTR-S	.20000+02	.10958+01	-.03735+00	.18764+01
FE	SGTR-S	.10000+02	-.60181+01	-.08151+01	.59566+01

Table 23. An Ellipsoidal Fit to Study the Influence of Different Types of Integral Data BLACK.DK09CF-3G-FE with 3 Groups, 24 Unknowns, 9 k Values, and 9 Reaction Rate Ratios

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********** 3 GROUP: ELLIPSOIDAL CONSTRAINT **********
                              .1TH GAMMA = .12964+00
ERROR IN K = .50000-02      SYSTEM ERROR = .00000
IN ASSLY 31,32,33,34,35,36,37,39,40,
ERROR IN PU240 CAPT/PU239 FTS = .70000-01   SYSTEM ERROR = .00000
IN ASSLY 31,32,33,34,35,36,37,39,40,
DELTA = .25000+01  FM = .77649+00  ASD = .76337+00  AD =-.14167-01
```

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAP1	.50000+01	-.12810+01	.54144-02	.23954-01
PU240	SGCAP1	.10000+02	.12934+02	-.10101+01	.98904+00
FE	SGCAP1	.20000+02	-.42810+02	-.29003+00	.17807+01
PU239	SGFIS1	.30000+01	-.45835+01	-.10135+01	.10816+01
PU240	SGFIS1	.30000+01	.36410+00	.12405+00	.20999+01
PU239	SGTR-1	.20000+02	-.38580+01	-.83534+01	.15614+02
PU240	SGTR-1	.20000+02	-.94126+01	-.11740+01	.57049+01
FE	SGTR-1	.20000+02	.57636+01	-.30348+02	.16971+02
PU239	SGCAP2	.50000+01	-.45824+01	.27600+00	.50666+00
PU240	SGCAP2	.10000+02	-.84593+00	-.12793+01	.67902+01
FE	SGCAP2	.20000+02	-.43235+01	-.37161+01	.93096+01
PU239	SGFIS2	.30000+01	.20664+01	.28909+01	.15664+01
PU240	SGFIS2	.30000+01	-.11092+01	.97277+00	.83451+00
PU239	SGTR-2	.15000+02	.91247+01	-.92159+01	.11552+02
PU240	SGTR-2	.20000+02	-.27542+02	-.31265+01	.11839+02
FE	SGTR-2	.20000+02	-.26520+02	-.11417+02	.98706+01

Table 23. Concluded

ISOTOPE NAME	CROSS SECTION ERROR TYPE	STD-DEV OF CROSS SECTION IN PERCENT	KNOWN ERROR IN PERCENT	ERROR IDENTIFIED IN PERCENT	STD-DEV OF IDENTIFIED ERROR IN PERCENT
PU239	SGCAPS	.50000+01	.38082+01	-.79655+00	.22808+01
PU240	SGCAPS	.10000+02	-.11418+01	-.73237+01	.58150+01
FE	SGCAPS	.10000+02	-.95346+01	-.53534+01	.80450+01
PU239	SGFISS	.50000+01	.12190+01	-.02694+01	.32342+01
PU240	SGFISS	.30000+01	-.15672+01	-.47755-02	.73542-02
PU239	SGTR-S	.10000+02	-.25208+01	-.11157+01	.95405+00
PU240	SGTR-S	.20000+02	.10958+01	-.07981+01	.20162+01
FE	SGTR-S	.10000+02	-.60181+01	.74589+01	.49362+01

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